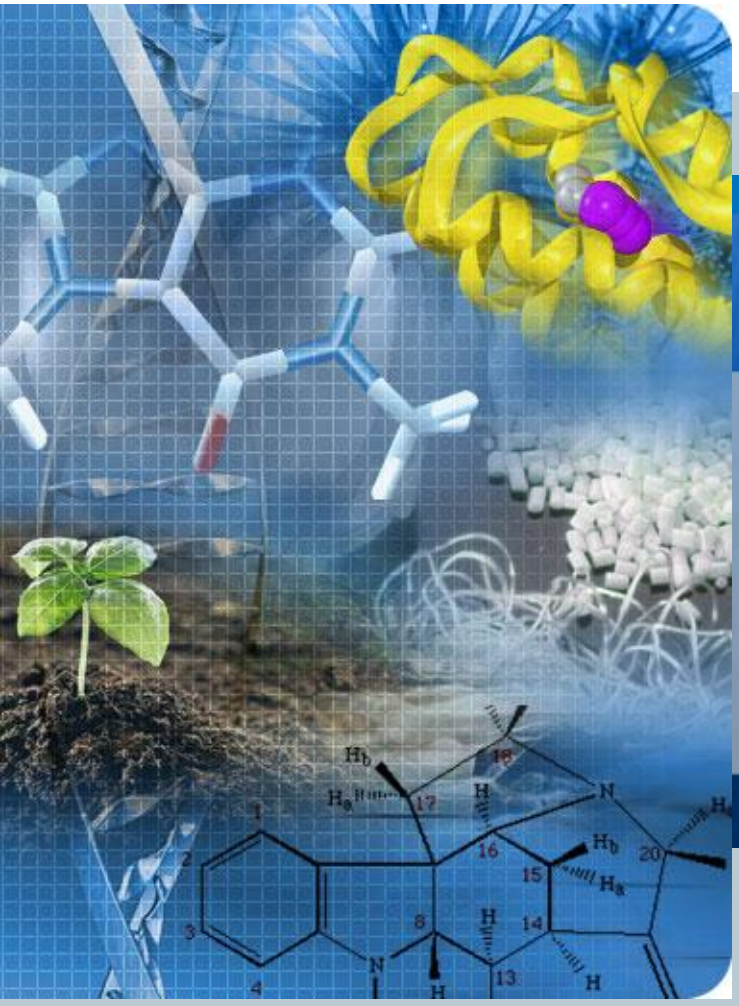
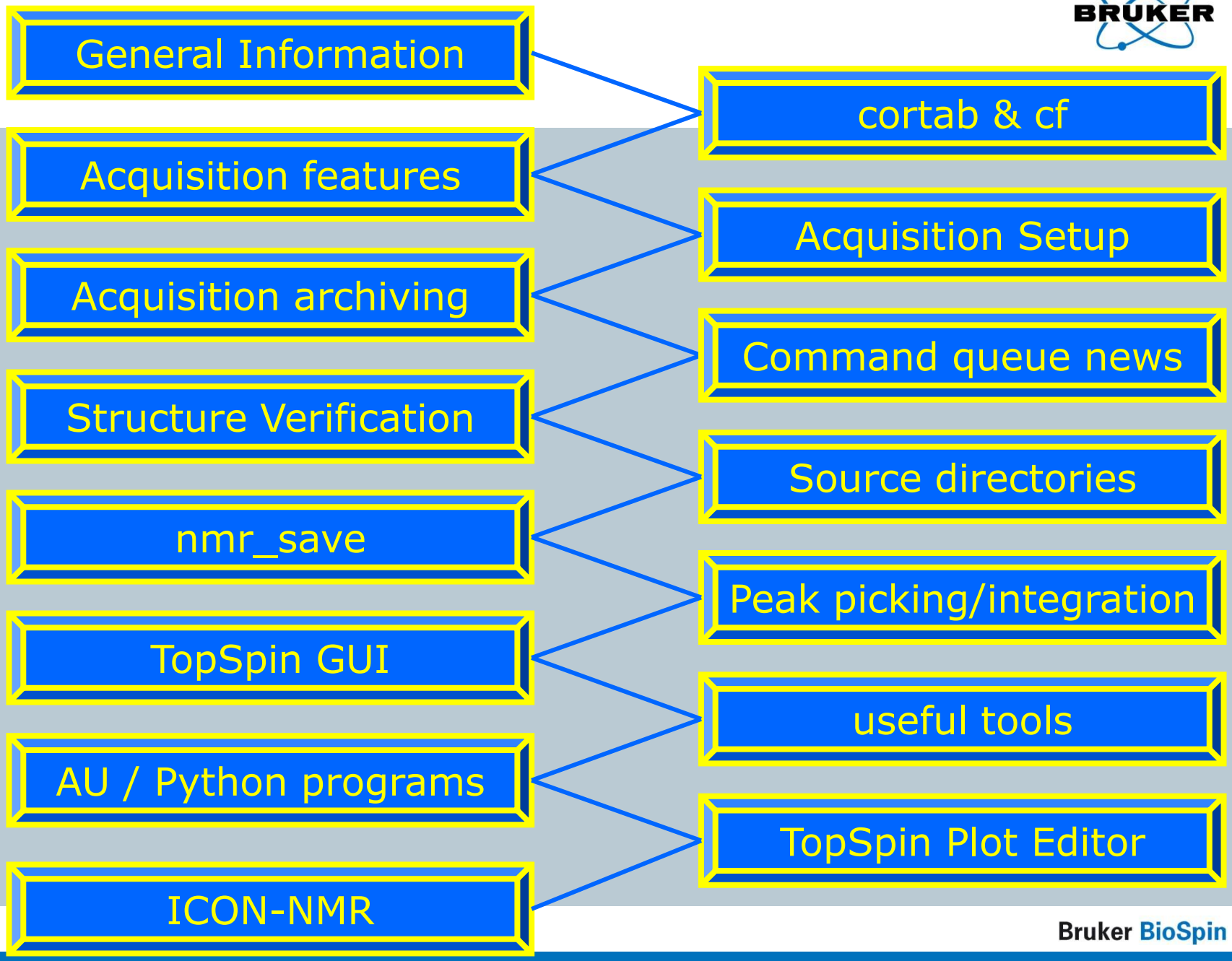


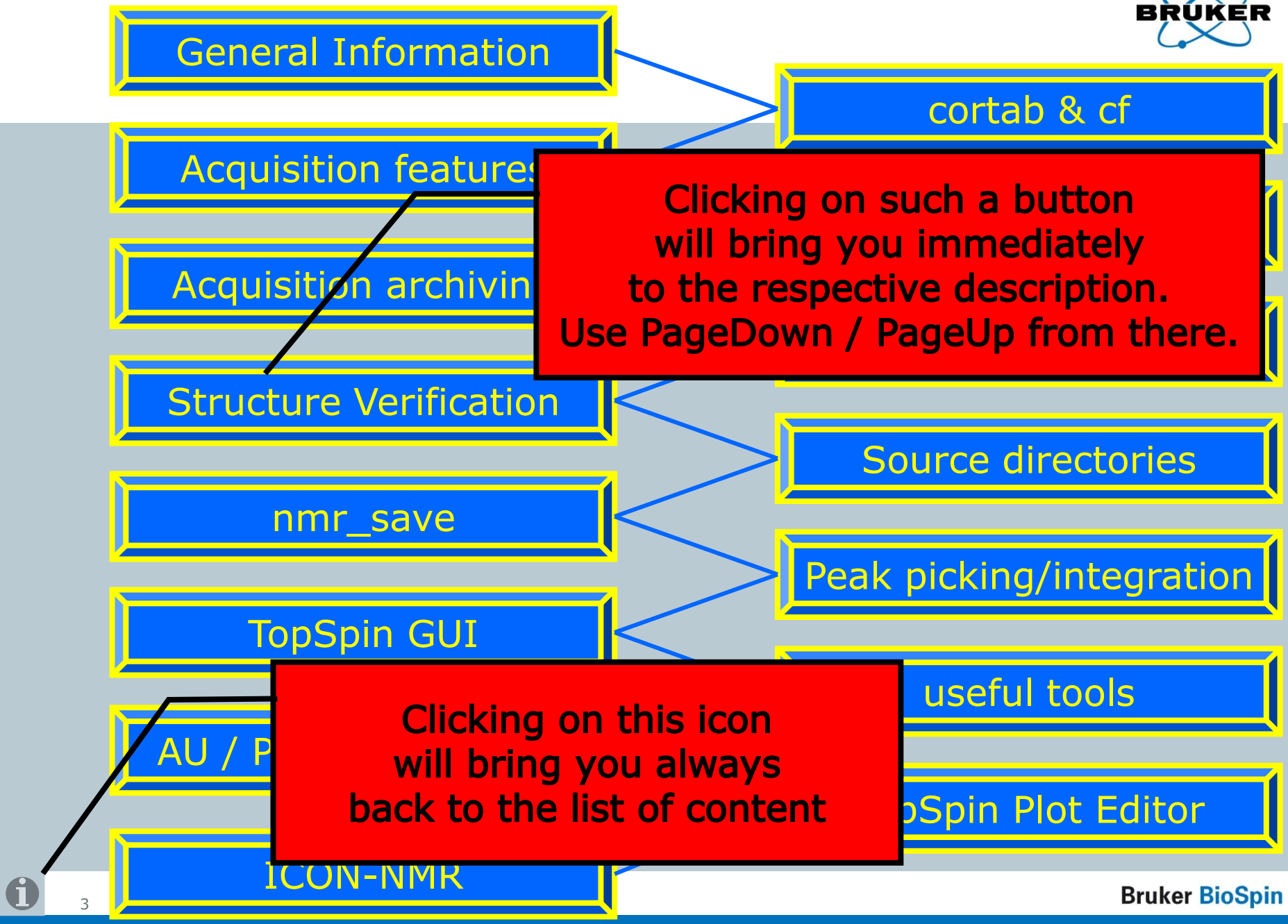
Release Letter TopSpin 2.1

Picture Presentation

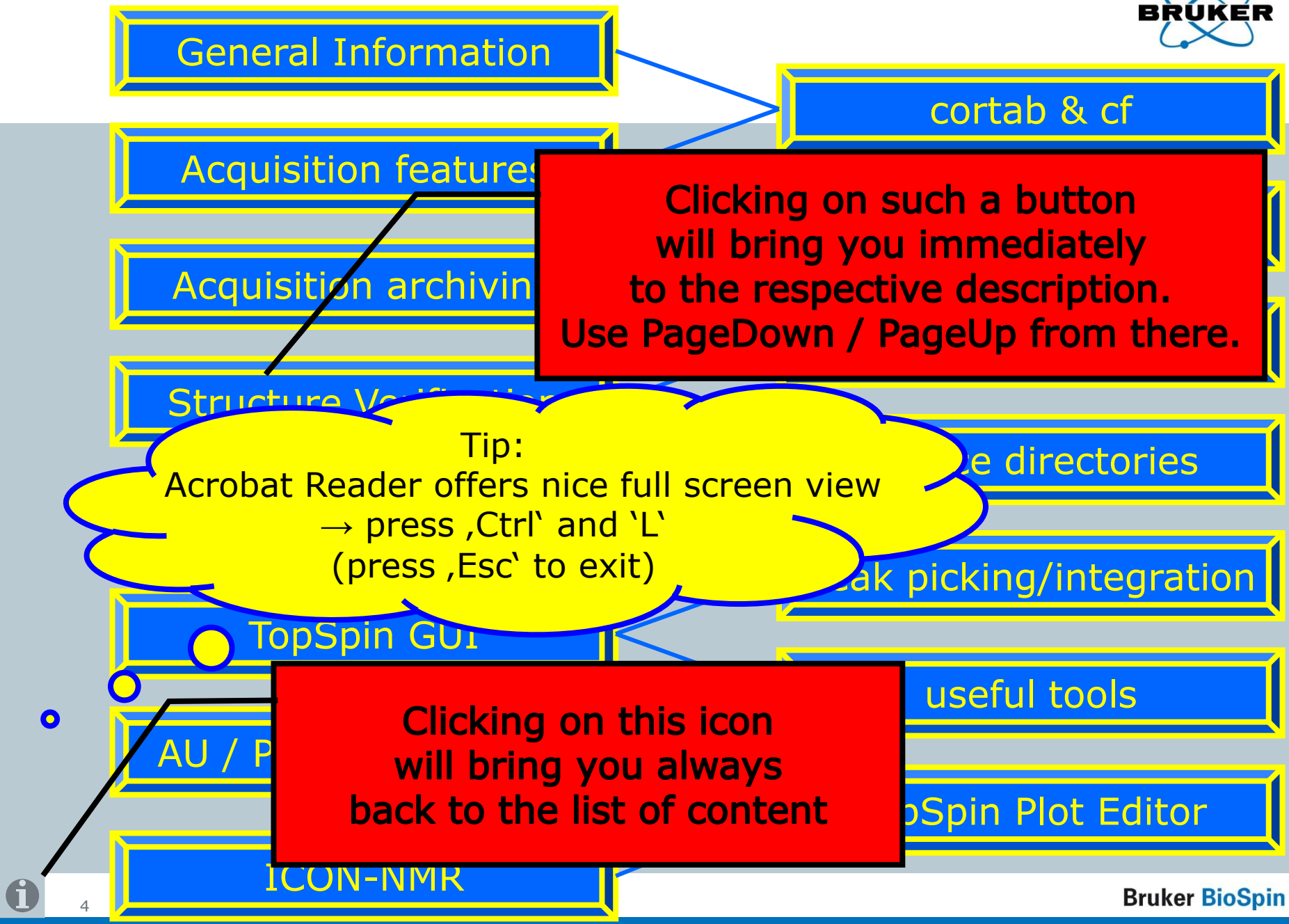
Content


General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

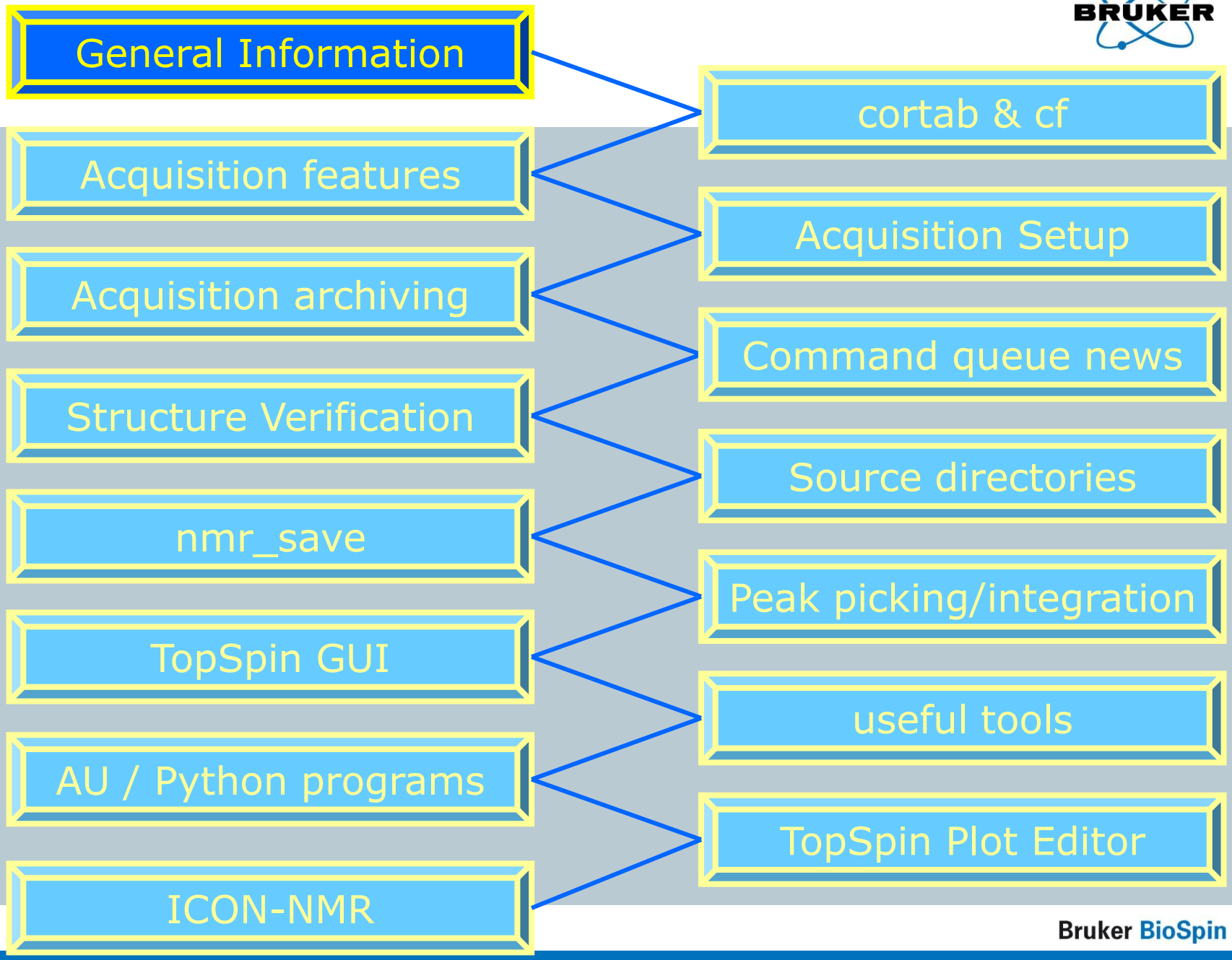
How to use this document



How to use this document



Content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Spectrometer support - TopSpin

	Avance III	Avance II	Avance I	D*X
TopSpin 2.1	✓	✓	✓	-
TopSpin 2.0	✓	✓	✓	-
TopSpin 1.3	-	✓	✓	✓
TopSpin 1.2	-	-	✓	-
TopSpin 1.1	-	-	-	-

OS support - TopSpin 2.1

	RHEL WS 3	RHEL WS 4	RHEL WS 5	W2k	Win XP	Win Vista
Processing	✓	✓	✓	✓	✓	✓
Acquisition	✓	✓	-	-	✓	✓

32 bit version

Support – Spectrometer/TopSpin/OS

	D*X	AVI	AVII	AVIII
TopSpin 1.3	✓	✓	✓	✓
TopSpin 2.0	-	✓	✓	✓
TopSpin 2.1	-	✓	✓	✓
Windows 2000	✓	✓ (1.3)	✓ (1.3)	-
Windows XP	✓	✓	✓	✓
Windows Vista	-	✓ (2.1)	✓ (2.1)	✓ (2.1)
RHEL WS 3	✓	✓	✓	✓
RHEL WS 4	✓ (1.3pl6)	✓ (2.0)	✓ (2.0)	✓
RHEL WS 5	-	-	-	-

Licenses

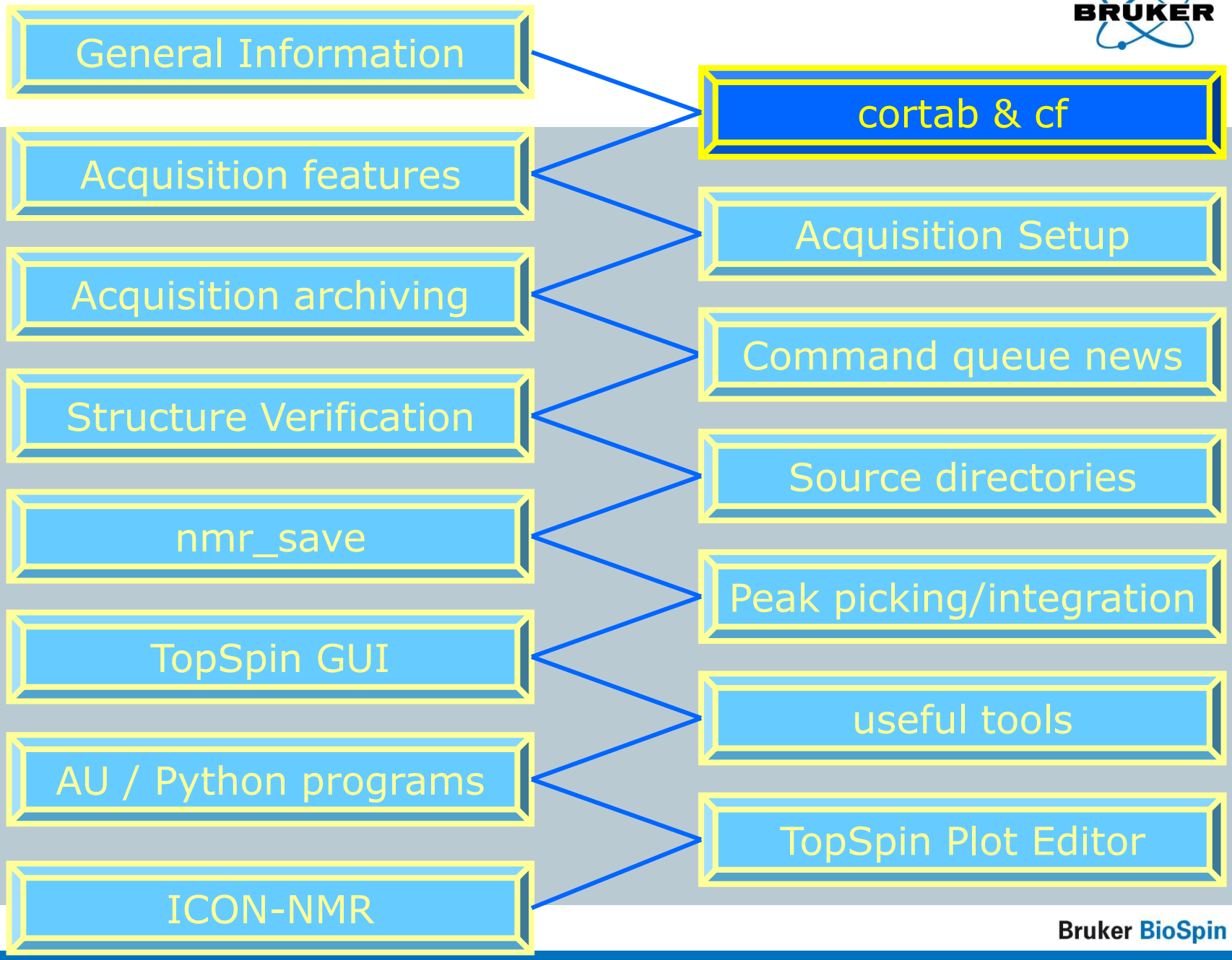
TopSpin 2.1 is a minor upgrade from 2.0

All you need is:

 a TopSpin 2.0 license

 a TopSpin 2.1 DVD

Content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Cortab news I

New procedure to correct
phase dependency of receiver gain

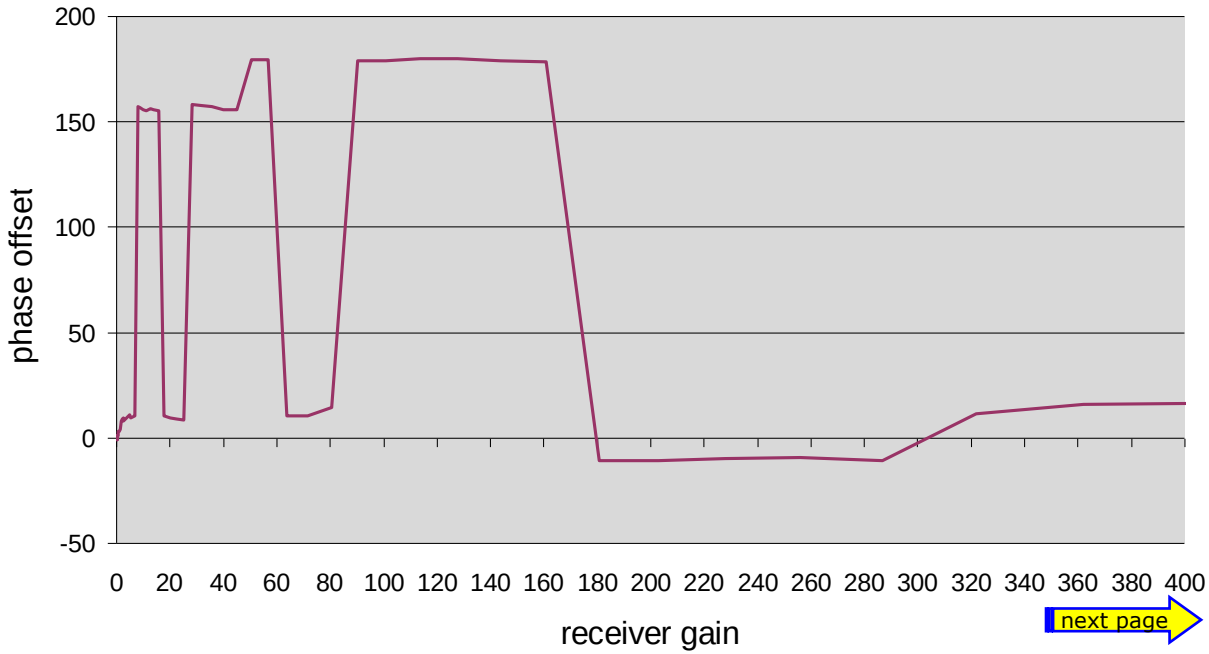
next page

Cortab news Ia

Because of the phase dependency of the RG value there is a phase offset if a 2D phasing is done on a basis of a 1D with different RG.

Cortab offers new functionality **REC Phase Linearization** which corrects this situation.

With TopSpin 2.1 the receiver phase correction should be done together with every new cortab.



Cortab news Ib

If the receiver gain adjustment for a certain nucleus fails during a multiple-experiment session (three experiments or more), the failed experiment will be skipped and the system continues with the next nucleus.

The skipped nuclei are collected an displayed at the end of the linearization procedure.

Cortab news II

New button that allows editing of amplifier peak power values in an existing cortab table.

Cortab news III

Cortab now allows the user
to set up a queue of experiments
easily and quickly.

cf news I

cf supports broad band type amplifier modules as BB (not X or H)

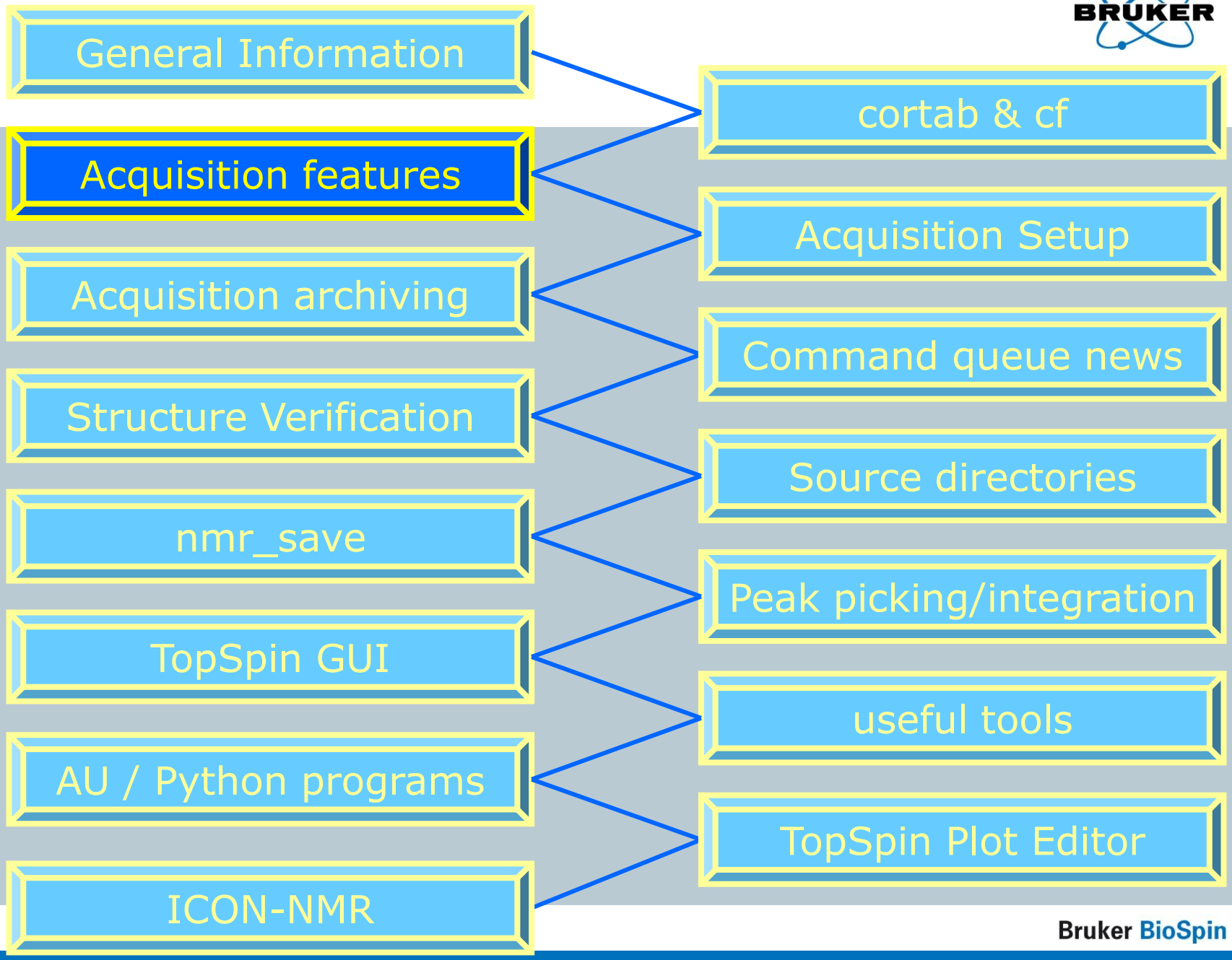
cf news II

cf supports 19F lockswitch

Wobble with switchbox

Wobble is now able to switch
the switchbox between Proton and 19F

Content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Pulse program
syntax enhancement - 1

The power setting after a shape pulse remains as it was in the last point of the shape.

In previous TOPSPIN versions this was reset to the default power of the channel where the shape was executed.

Pulse program
syntax enhancement - 2

go=nn cpd2:f2 finally do:f2

"**do**" (decoupler off) is no longer needed at the place where the "**go**" loops back to and in the code following

Pulse program
syntax enhancement - 3

Now power calculations like:

pl5=sp23; pl3=cnst23;

are possible

Pulse program
syntax enhancement - 4

cpd following cpd without '**do**' (decoupler off) in between

Pulse program
syntax enhancement - 5

Two new parameters:

PLSTRT and **PLSTEP**

enable the automatic replacement of setting the pulse power level via slow analog attenuators by fast and artifact free amplitude setting using the digital modulation of the SGU.

APSY

TopSpin 2.1 supports the fast NMR method APSY (Automated Projection Spectroscopy)

APSY can be started under:

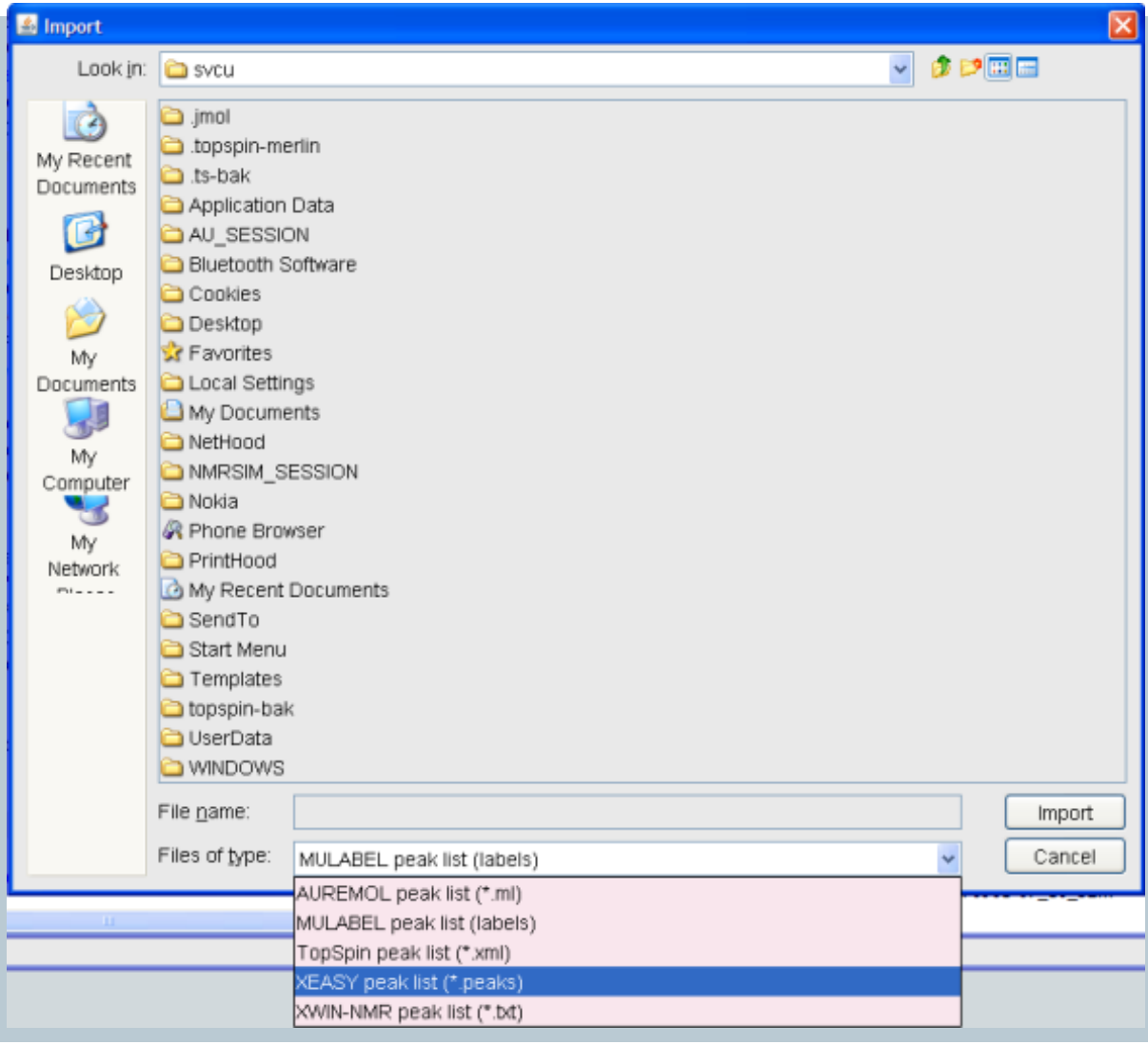
Spectrometer → Fast Acquisition Methods

APSY requires a separate license. A free demo license can be ordered anytime under: www.bruker-biospin.com

next page

XEASY peak list files can be im/exported

XEASY peak lists are the result of the fast NMR method **APSY**



Multiple Receiver

TopSpin 2.1 allows comfortable multiple receiver acquisition. Functionality of software routing has been enhanced by adding respective receiver setup.

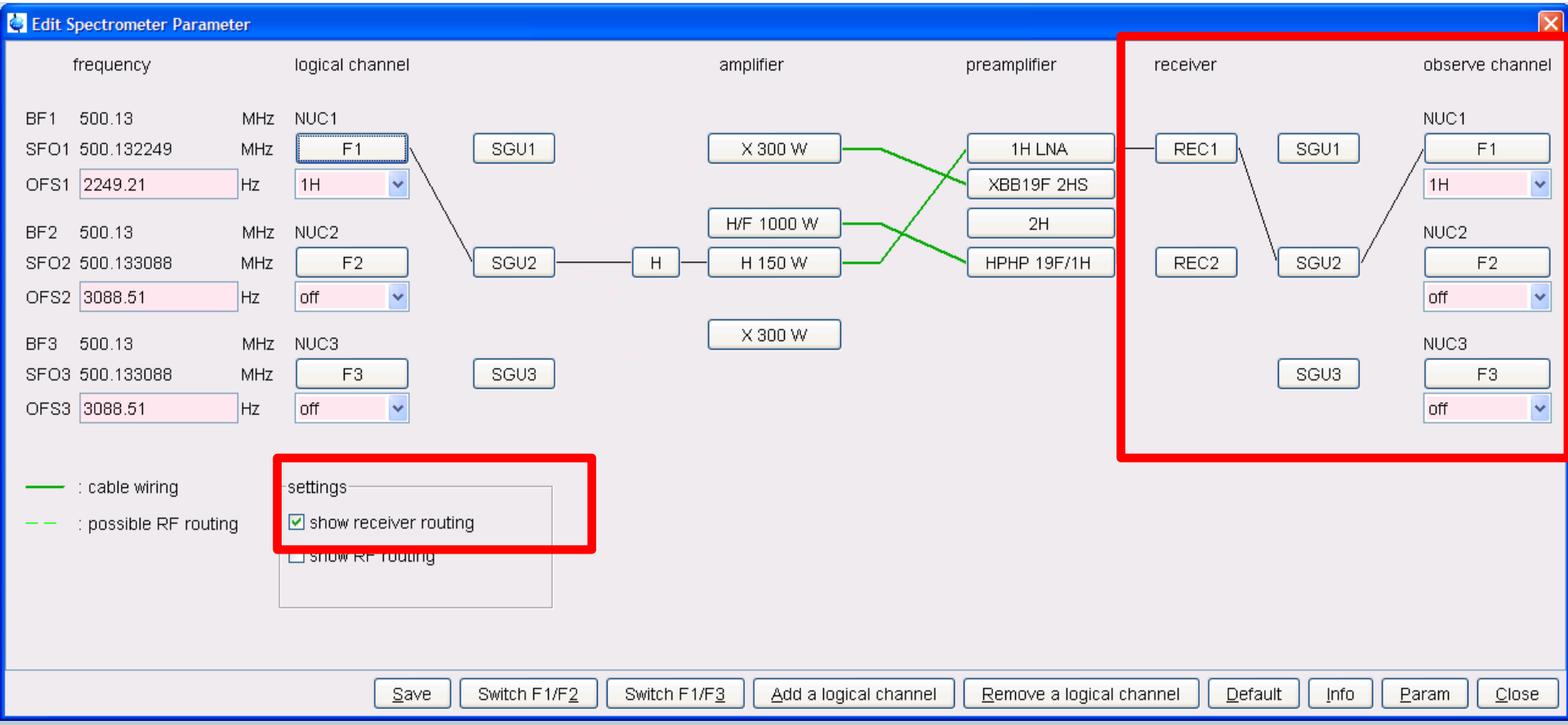
For detailed information enter

help AVIIIMultiReceive

in TOPSPIN 2.1 command line.

next page

Multiple Receiver



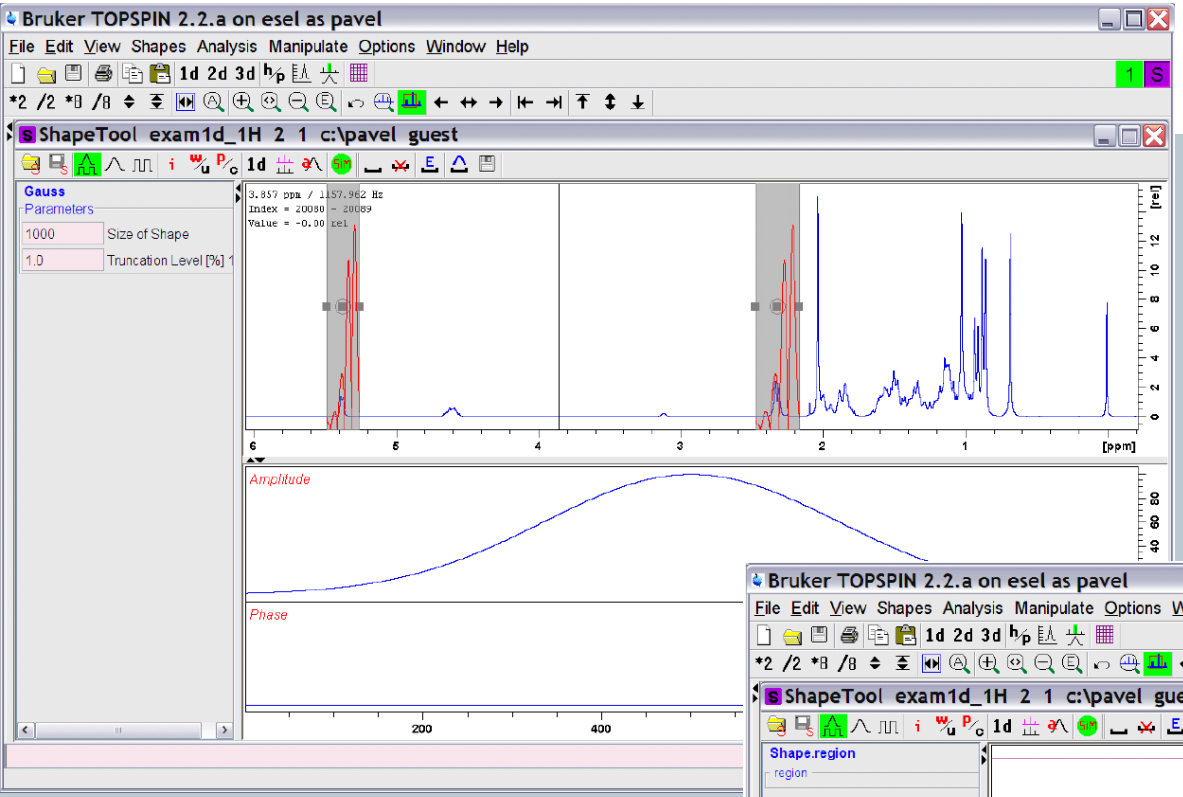
Shape tool – easy setup

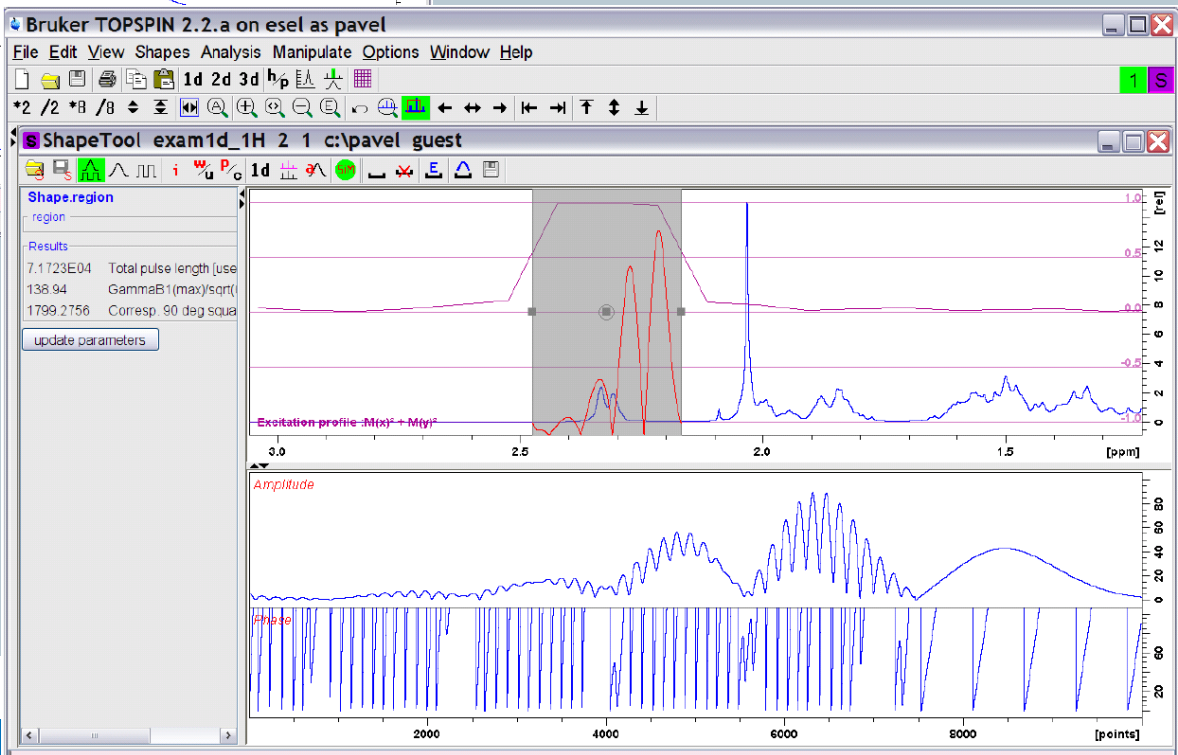
New feature allows interactive definition of excitation regions in Shape-Tool.

All parameters, such as power level, pulse length and the excited region, are coupled together for easy setup of selective experiments.

next page

Shape tool


Bruker TOPSPIN 2.2.a on esel as pavel
File Edit View Shapes Analysis Manipulate Options Window Help
ShapeTool exam1d_1H 2 1 c:\pavel guest
Gauss
Parameters
1000
Size of Shape
1.0
Truncation Level [%]
Amplitude
Phase
[ppm]


Bruker TOPSPIN 2.2.a on esel as pavel
File Edit View Shapes Analysis Manipulate Options Window Help
ShapeTool exam1d_1H 2 1 c:\pavel guest
Shape.region
region
Results
update parameters
Excitation profile: M(x)² + M(y)²
Amplitude
Phase
[ppm]
[points]

Eretic

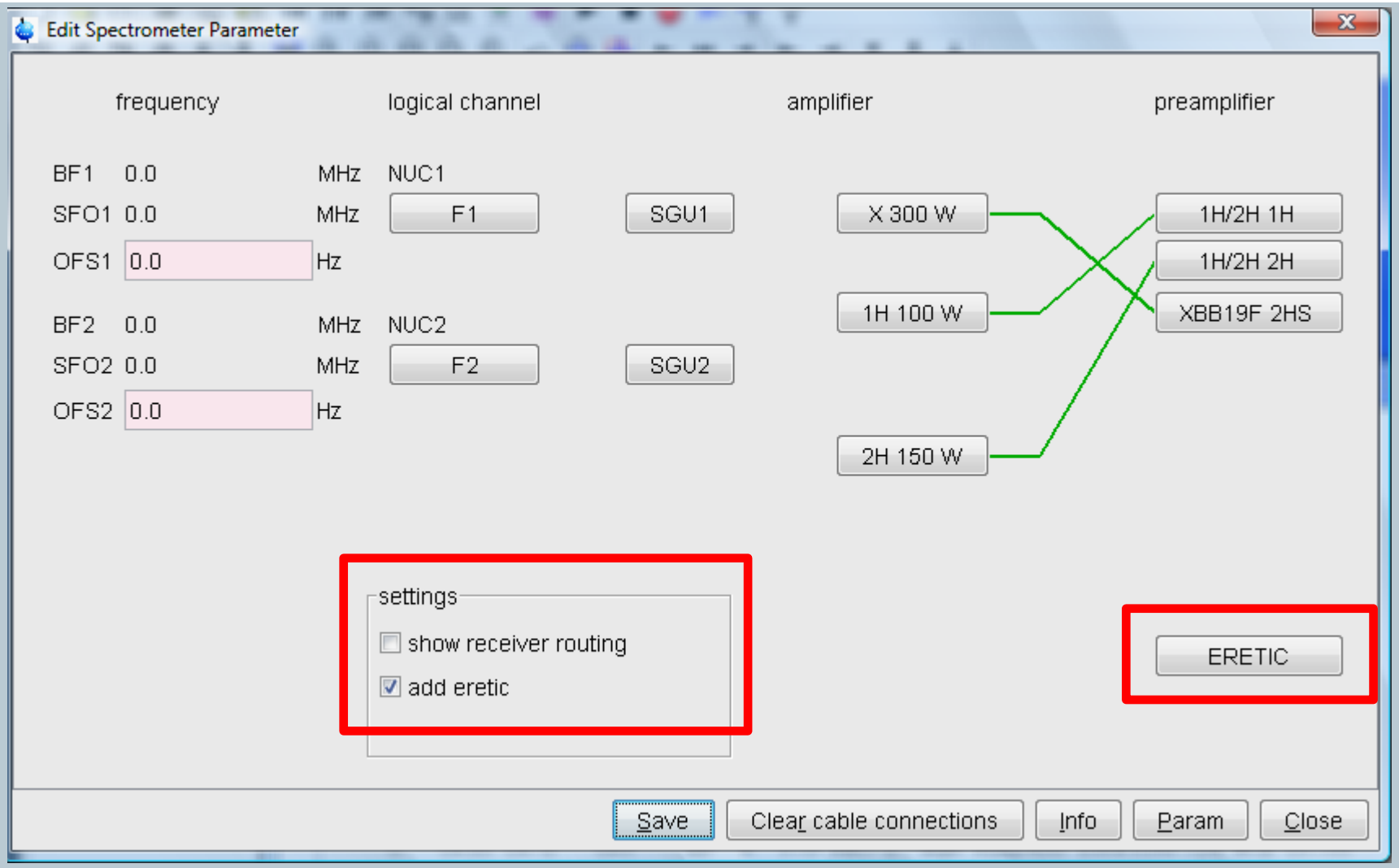
The Eretic channel can be defined during spectrometer configuration.

Eretic setup is now enabled for all AVANCE systems by the command

edasp

next page

Eretic


Edit Spectrometer Parameter
frequency
logical channel
amplifier
preamplifier
BF1 0.0 MHz NUC1
SFO1 0.0 MHz F1 SGU1
OFS1 0.0 Hz
BF2 0.0 MHz NUC2
SFO2 0.0 MHz F2 SGU2
OFS2 0.0 Hz
X 300 W
1H 100 W
2H 150 W
1H/2H 1H
1H/2H 2H
XBB19F 2HS
settings
show receiver routing
add eretic
ERETIC
Save
Clear cable connections
Info
Param
Close

paropt

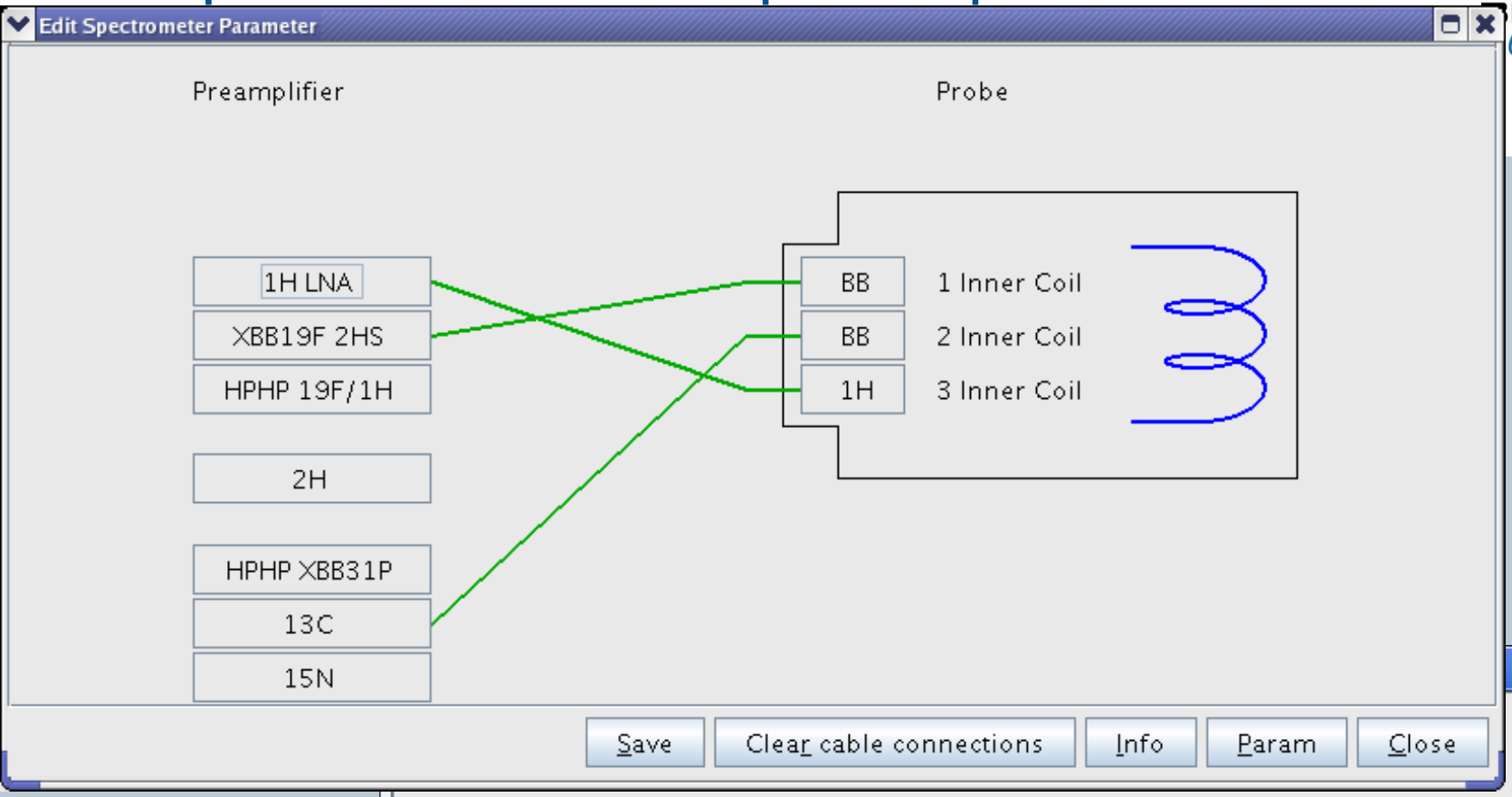
paropt can now be stopped
with the command **stop**

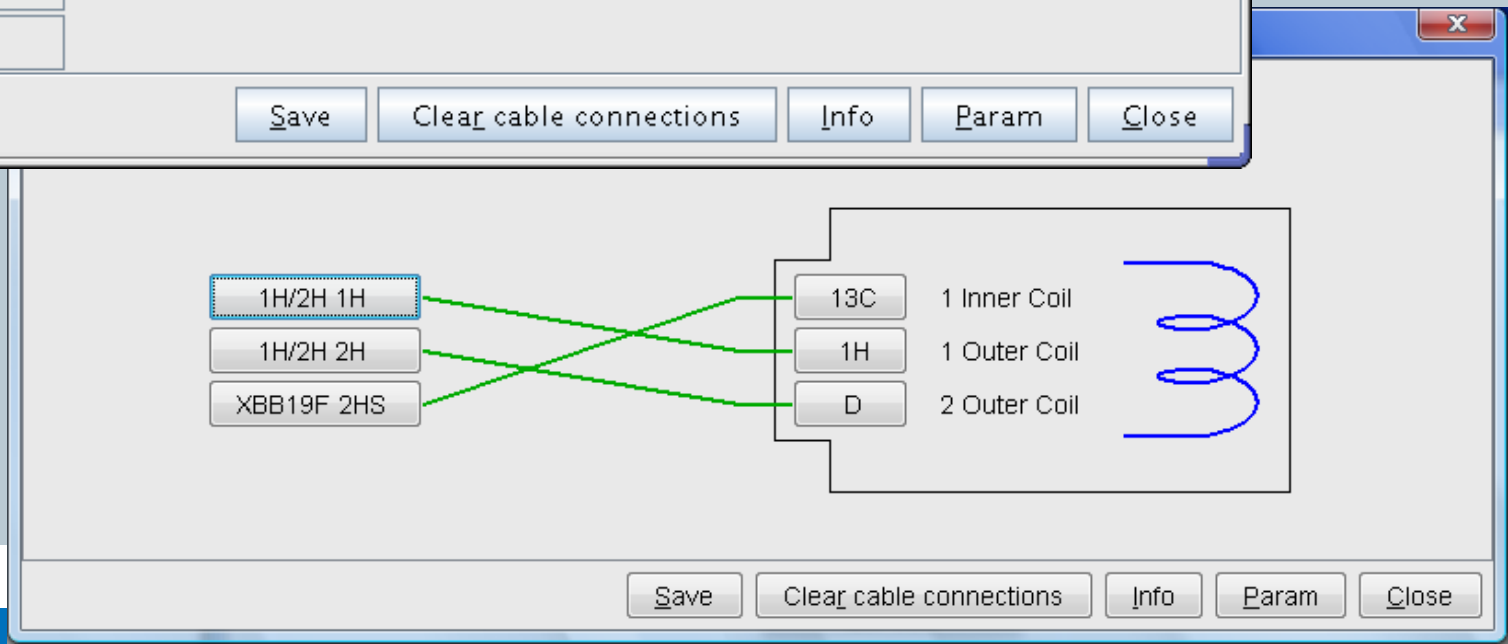
Edhead preamp connection

When exiting **edhead** it displays a new window where the preamp-probe connection can be defined.
This is used for power check to find out the correct peak power limit of the probe
(e.g. in case of a TBI probe for the 13C selective input or the BB input, respectively).

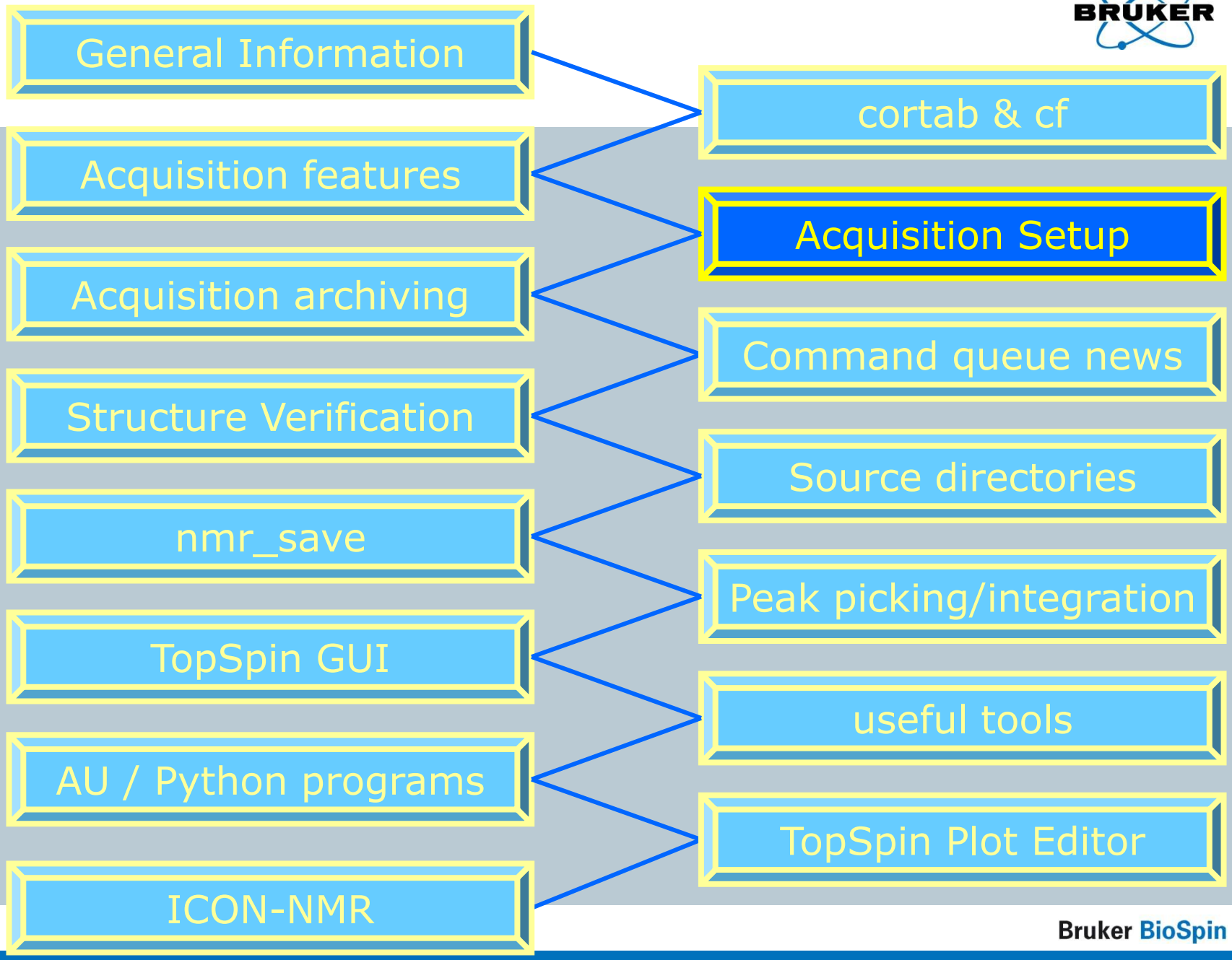
next page

Examples for **edhead** preamp connection





Content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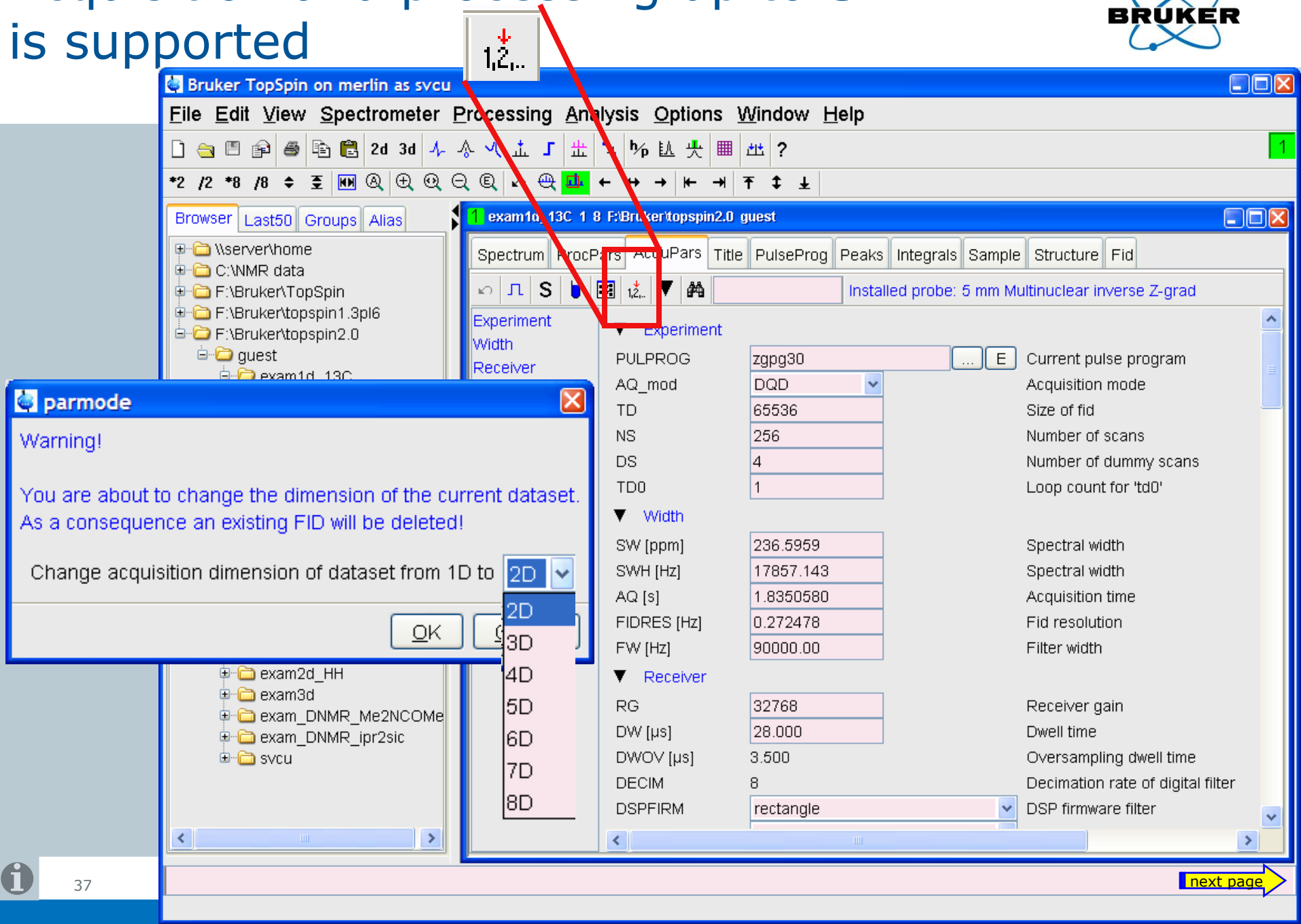
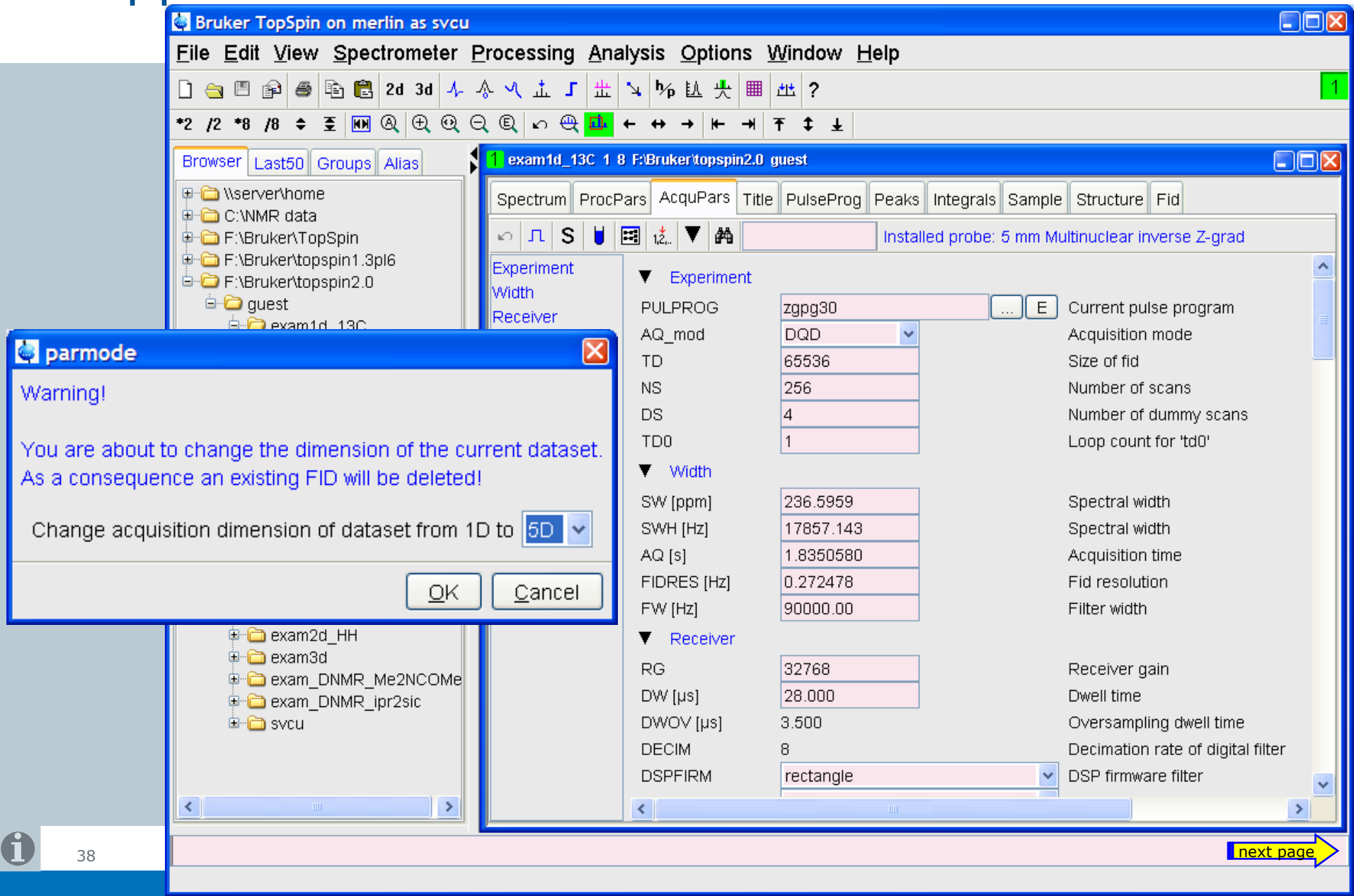
Acquisition and processing up to **8D** is supported



Acquisition and processing up to **8D** is supported



next page

Acquisition and processing up to **8D** is supported

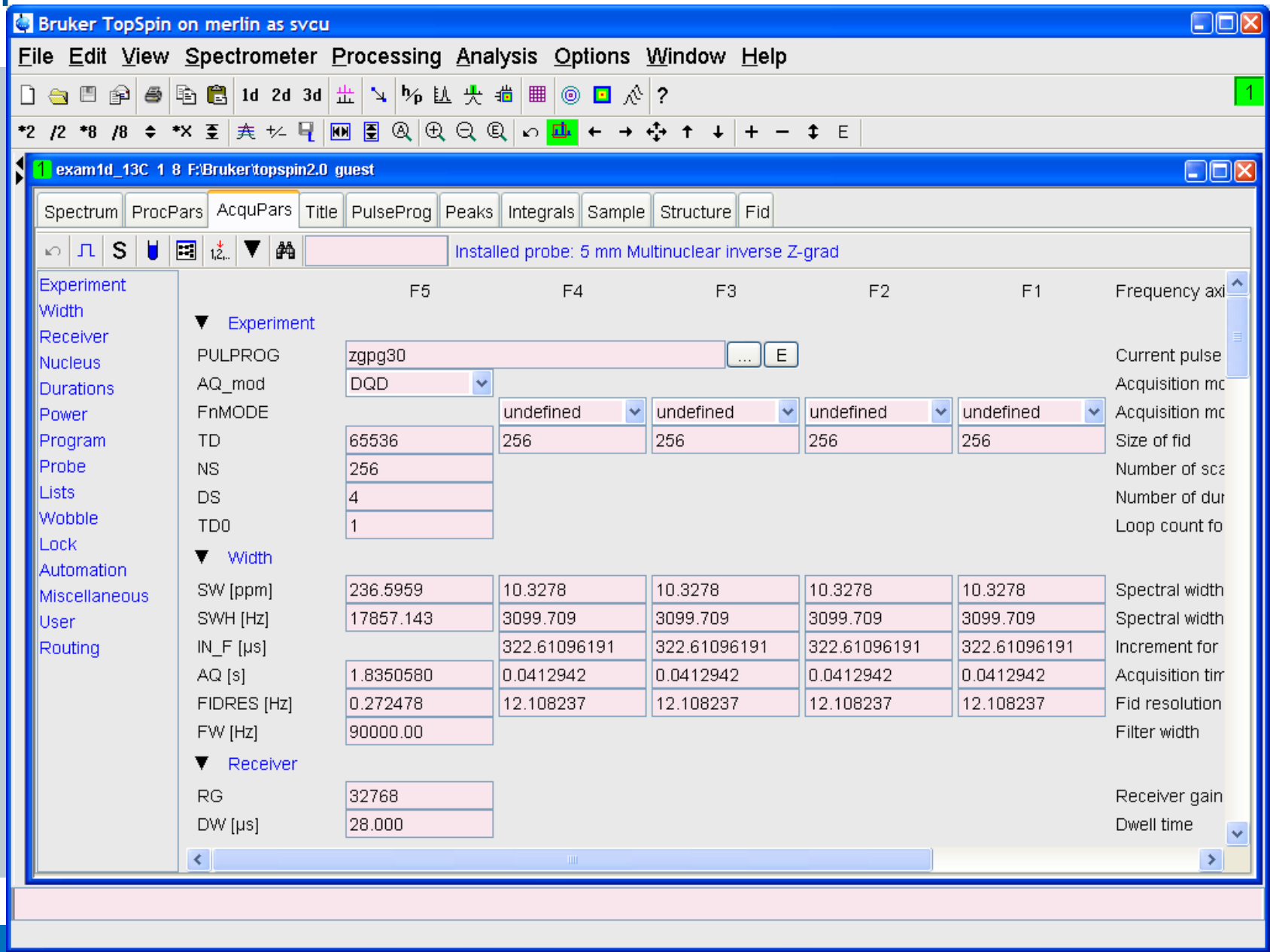
TopSpin 2.1 now provides examples for 4D experiments (HSQC-NOESY-HSQC):

- 4D parameter sets (ending with 4D)

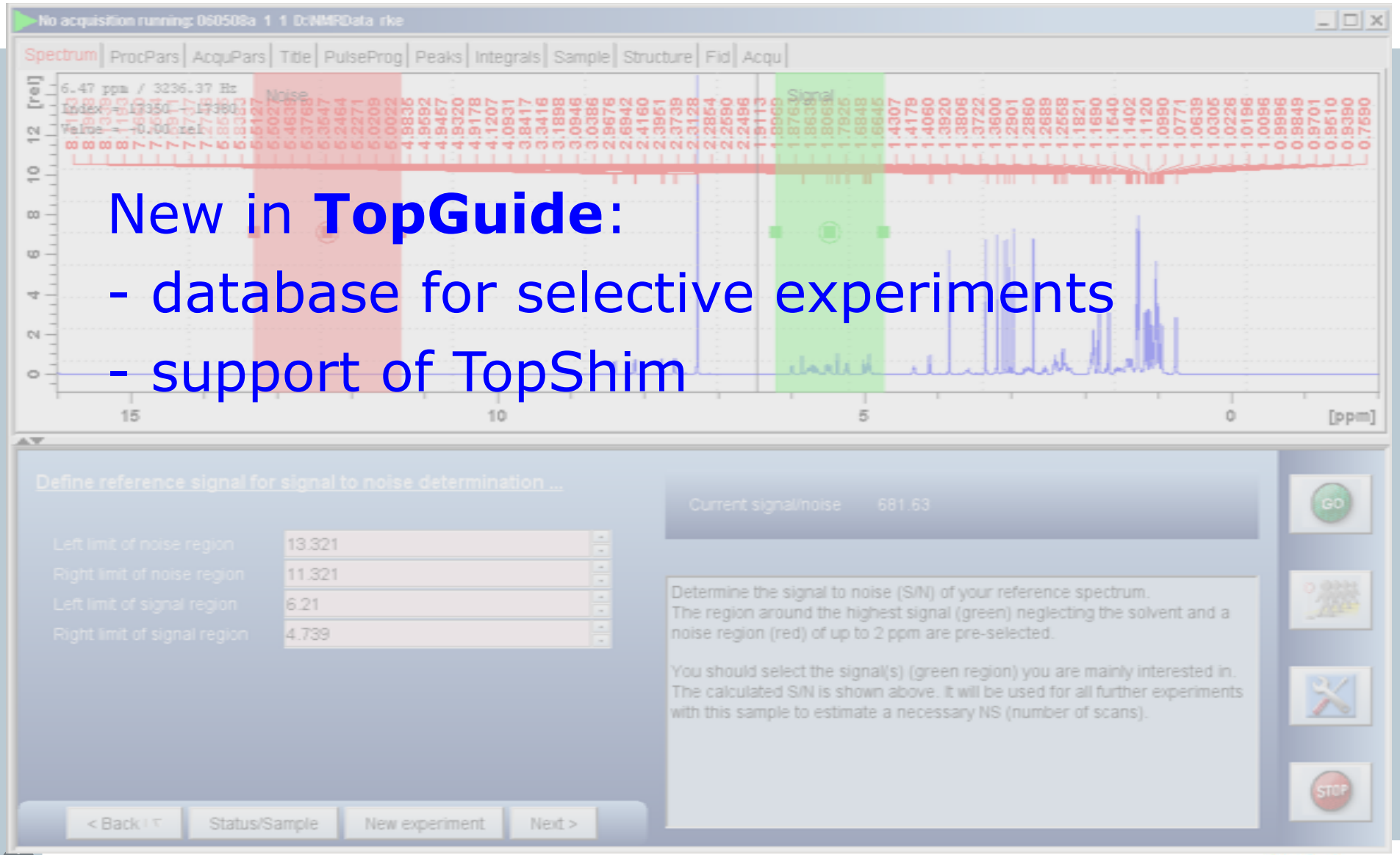
and

- 4D pulse programs (ending with 4d).

Acquisition and processing up to **8D** is supported



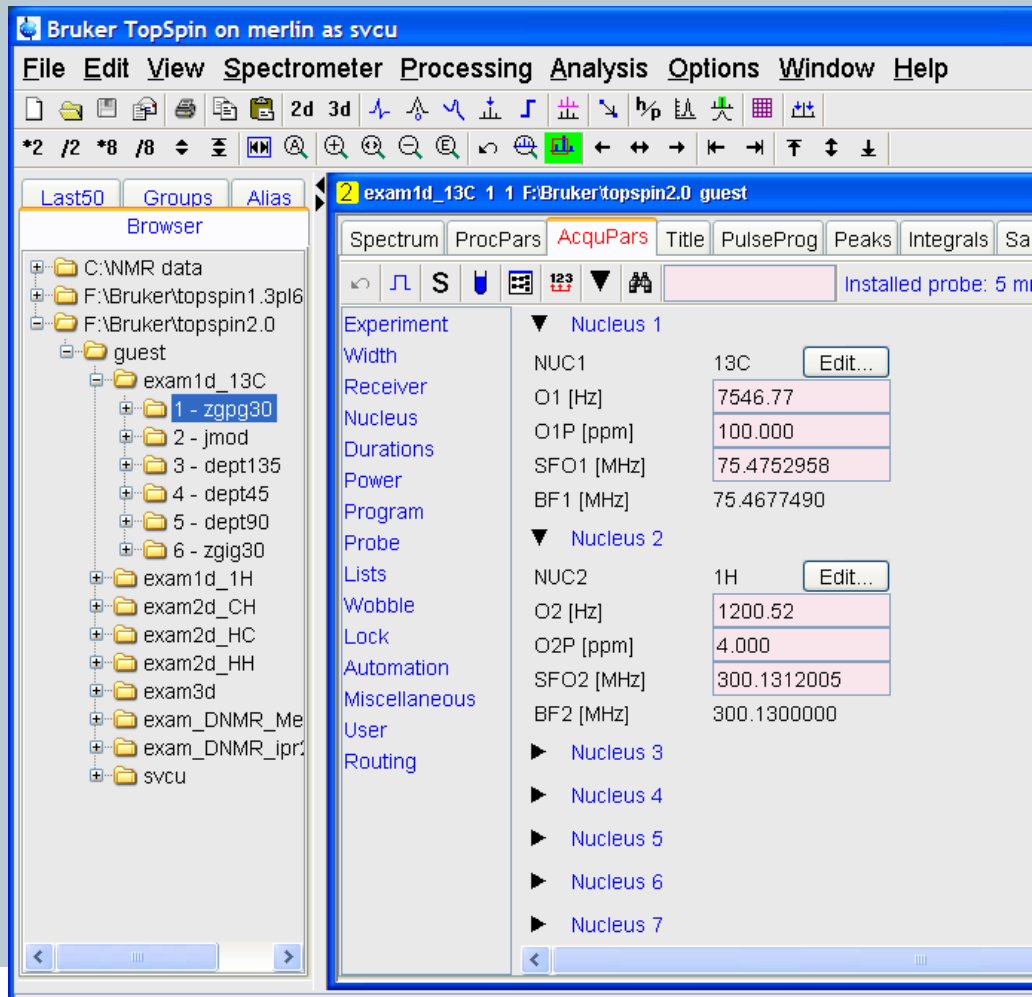
TopGuide News



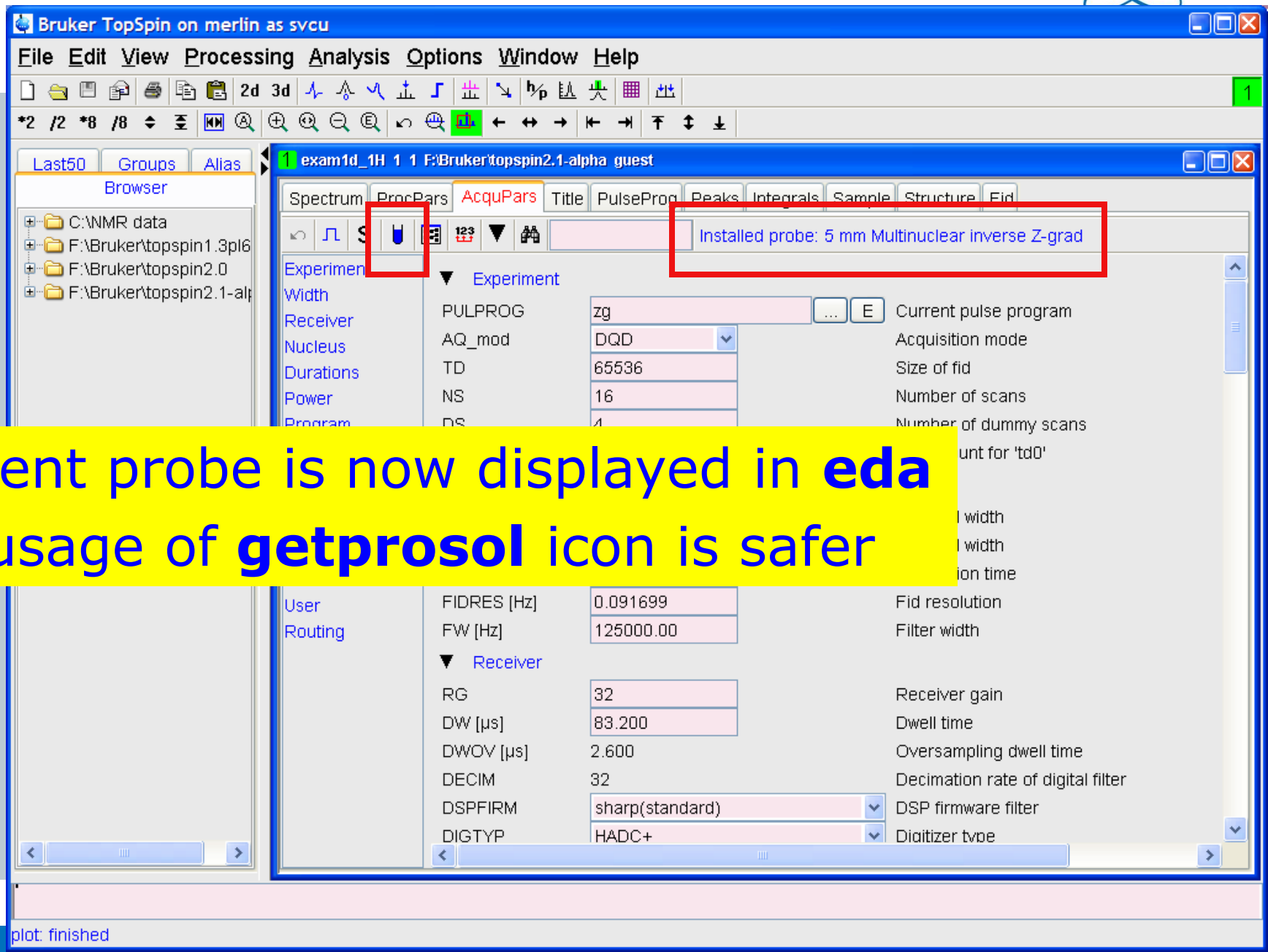
Acquisition parameters

Only these nuclei are shown which are used in the pulse program.
All others are collapsed automatically.

^{13}C {^{1}H}



Current probe



Current probe is now displayed in **eda**

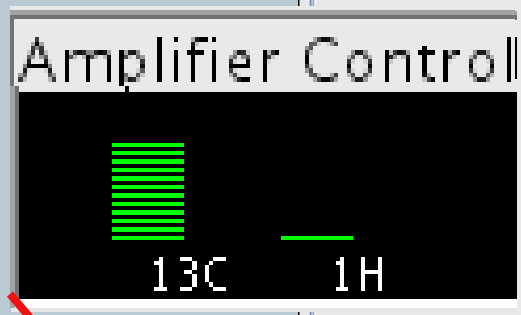
➔ usage of **getprosol** icon is safer

Amplifier status monitor

A status monitor is available for external amplifiers on Avance III systems.

next page

Amplifier status monitor



Bruker TOPSPIN 2.1.a on titanic as nmrsu

File Edit View Spectrometer Processing Analysis Options Window Help

Groups Alias
Browser Last50
/opt/ts20pl3

ACQ: es 1 1 /opt/alpha es

Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Fid Acqu

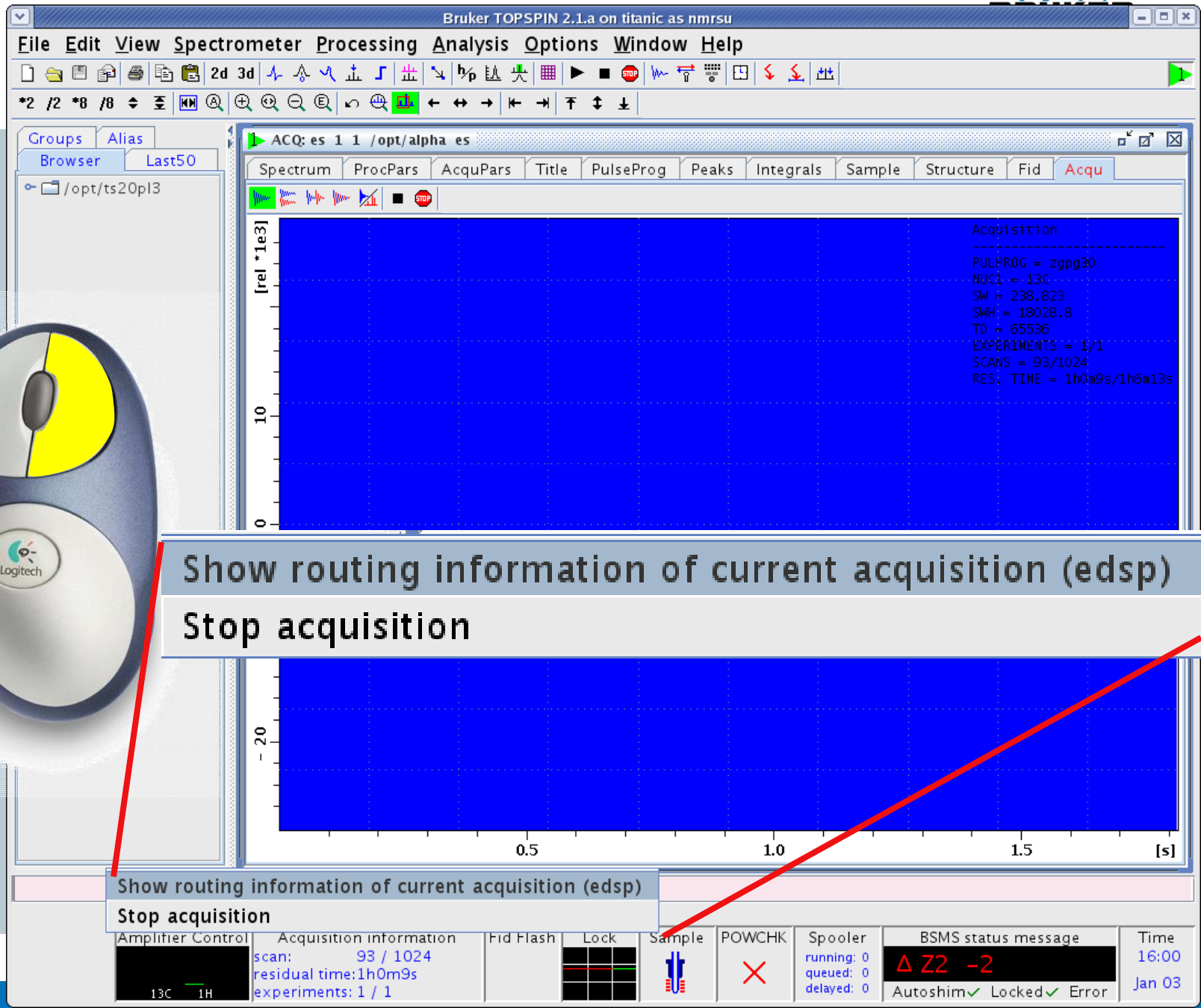
File: zgpg30 (/opt/alpha/exp/stan/nmr/lists/pp/user)

```
;$CLASS=HighRes
;$DIM=1D
;$TYPE=
;$SUBTYPE=
;$COMMENT=


;$OWNER=Bruker
#include <Avance.incl>
#include <Delay.incl>


"d11=30m"


"DELTA=d1-100m"


1 ze
  d11 pl12:f2
2 30m do:f2
  10u pl13:f2
  d11 cpd2:f2
  DELTA
  4u do:f2
  10u pl12:f2
  100m cpd2:f2
  p1*0.33 ph1
  go=2 ph31
  30m do:f2 pl13:f2 mc #0 to 2 F0(zd)
exit


ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

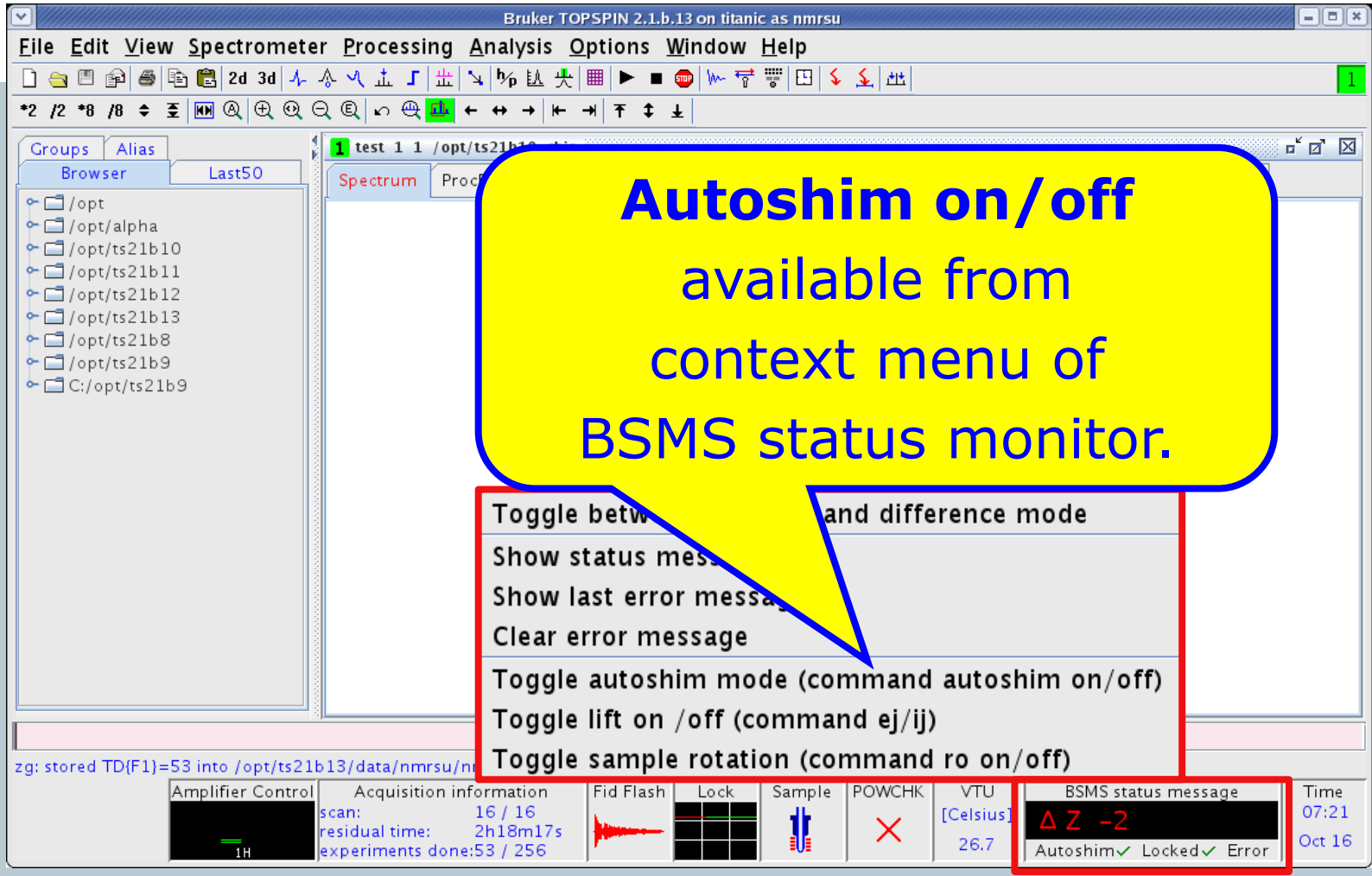
next page

Amplifier Control	Acquisition information	Fid Flash	Lock	Sample	POWCHK	Spooler	BSMS status message	Time
13C 1H	scan: 54 / 1024 residual time: 1h2m41s experiments: 1 / 1					running: 0 queued: 0 delayed: 0	Δ Z3 -3 Autoshim✓ Locked✓ Error	15:58 Jan 03

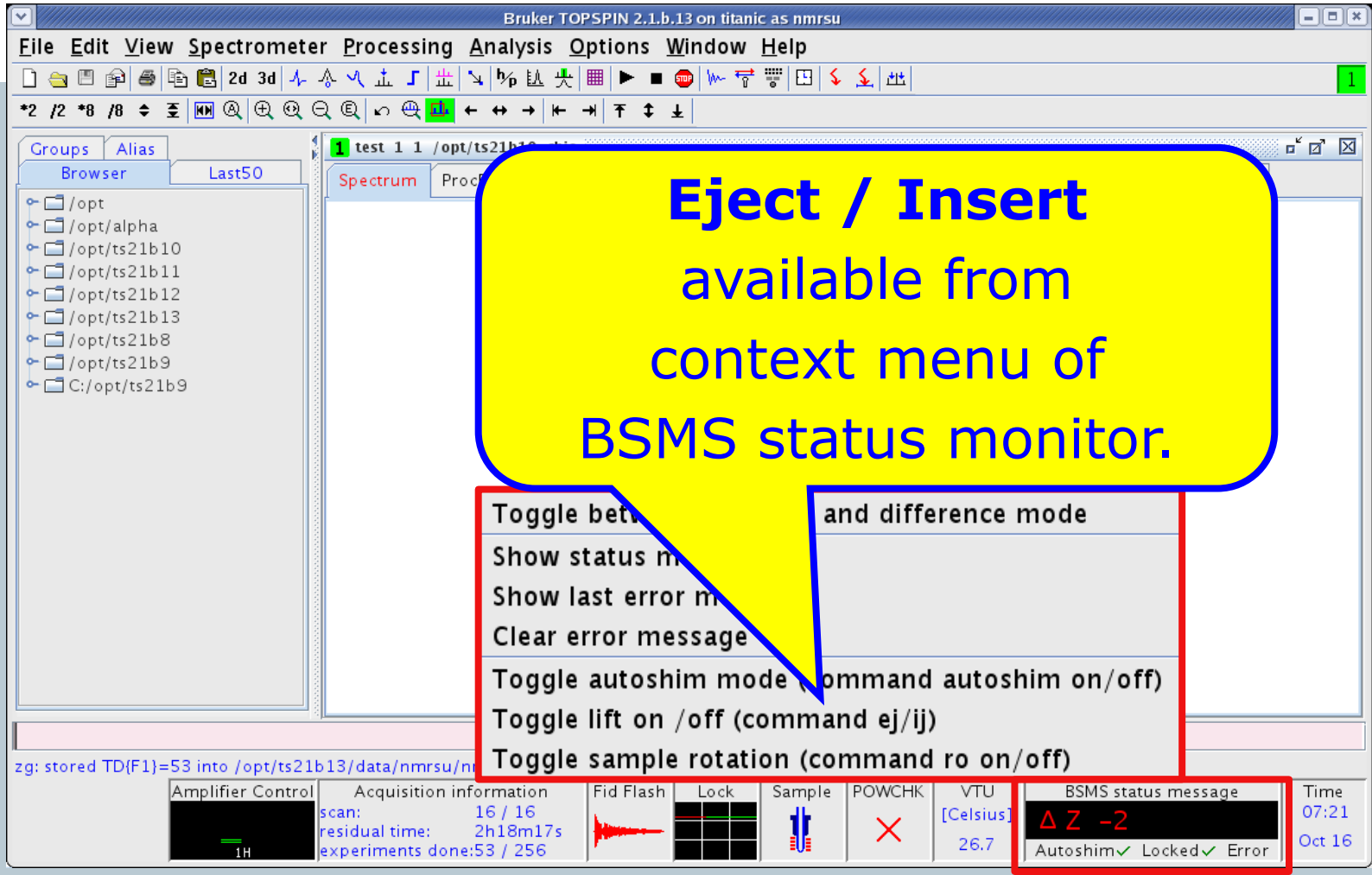
Amplifier status monitor



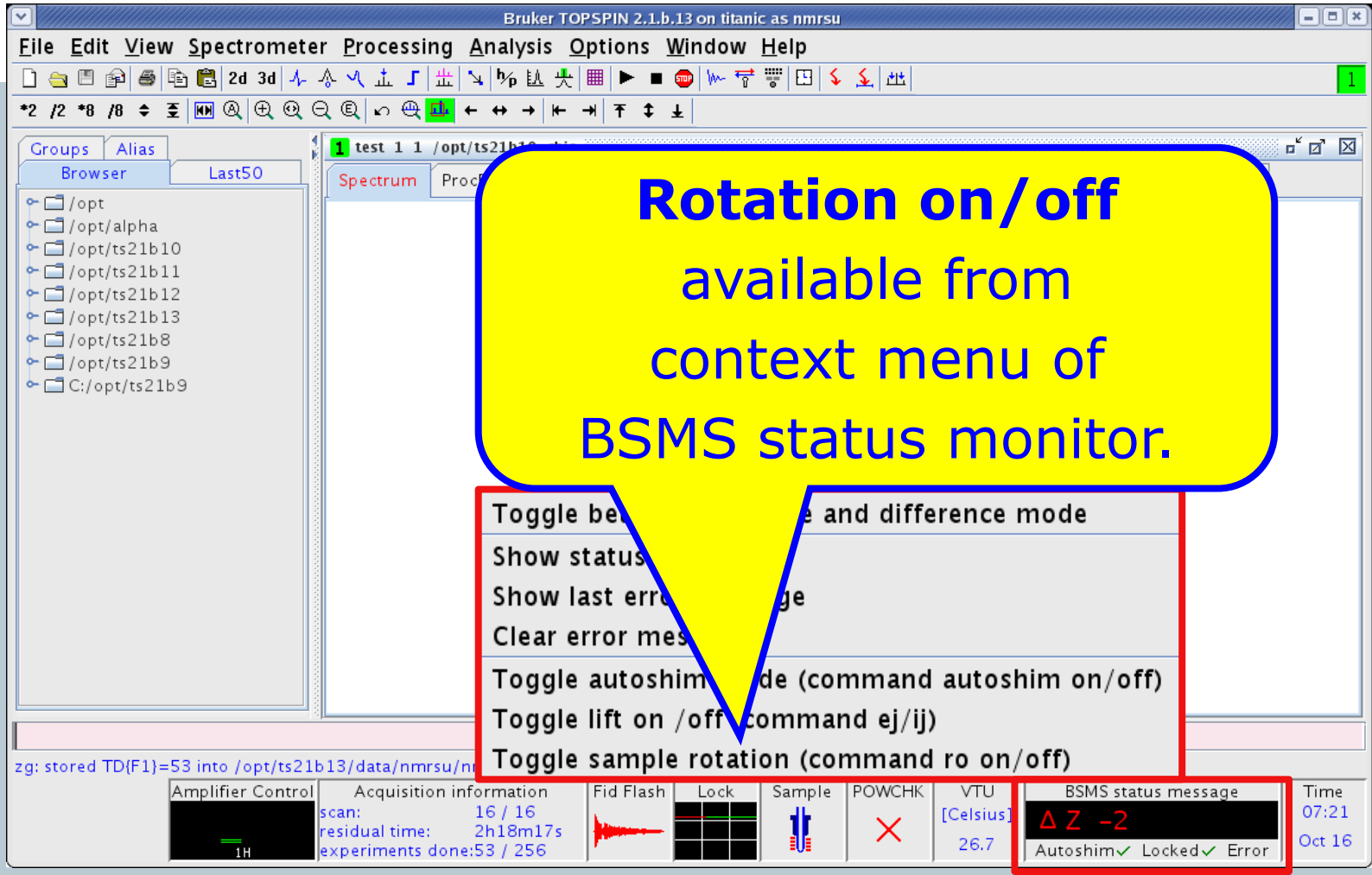
Autoshim on/off



Autoshim on/off



Autoshim on/off

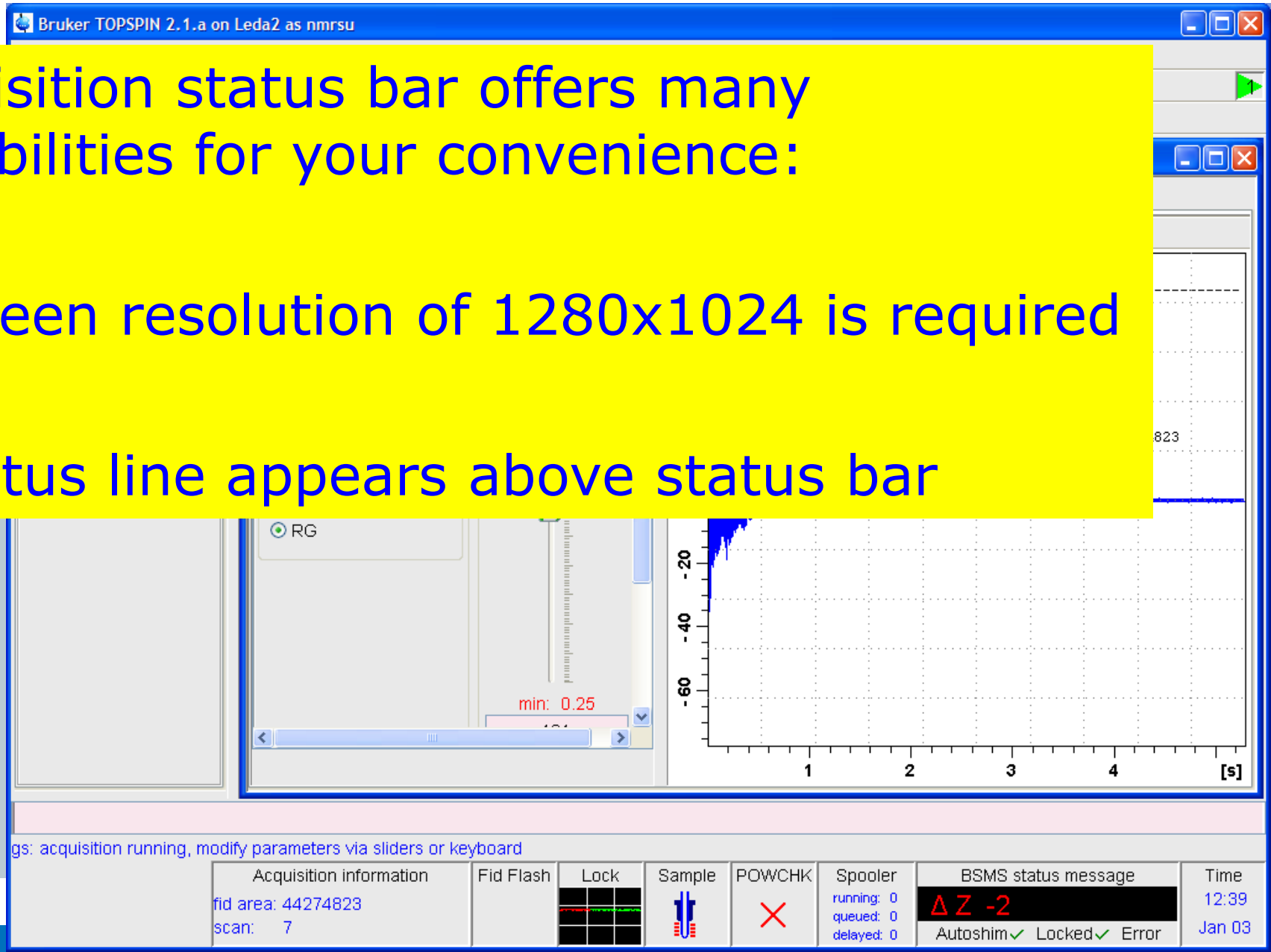


N2 sensor

BSMS display supports N2 sensor, if available.

The daily helium measurement will also check and protocol N2 if the N2 sensor is available.

command line / status bar

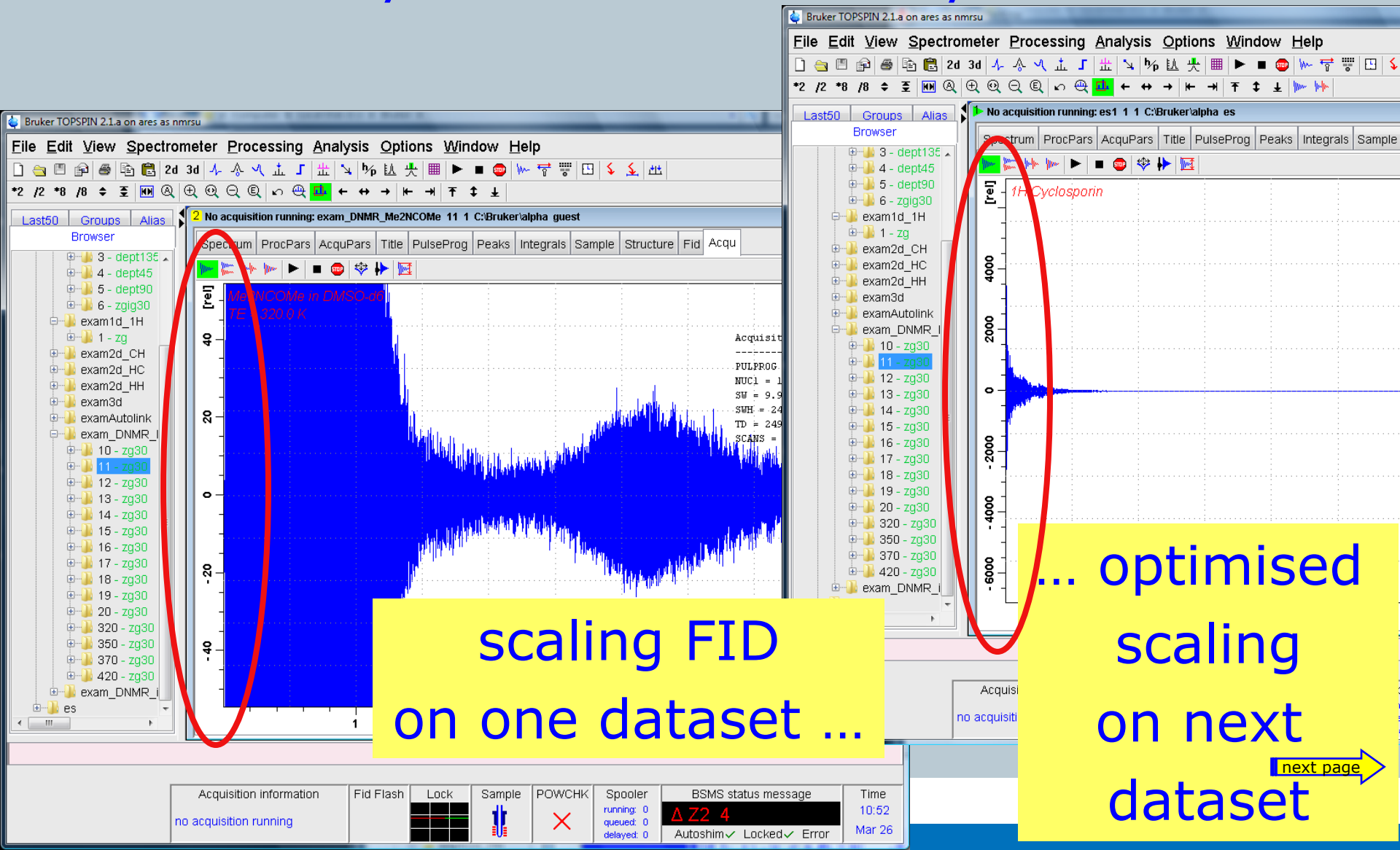


Acquisition status bar offers many possibilities for your convenience:

- screen resolution of 1280x1024 is required
- status line appears above status bar

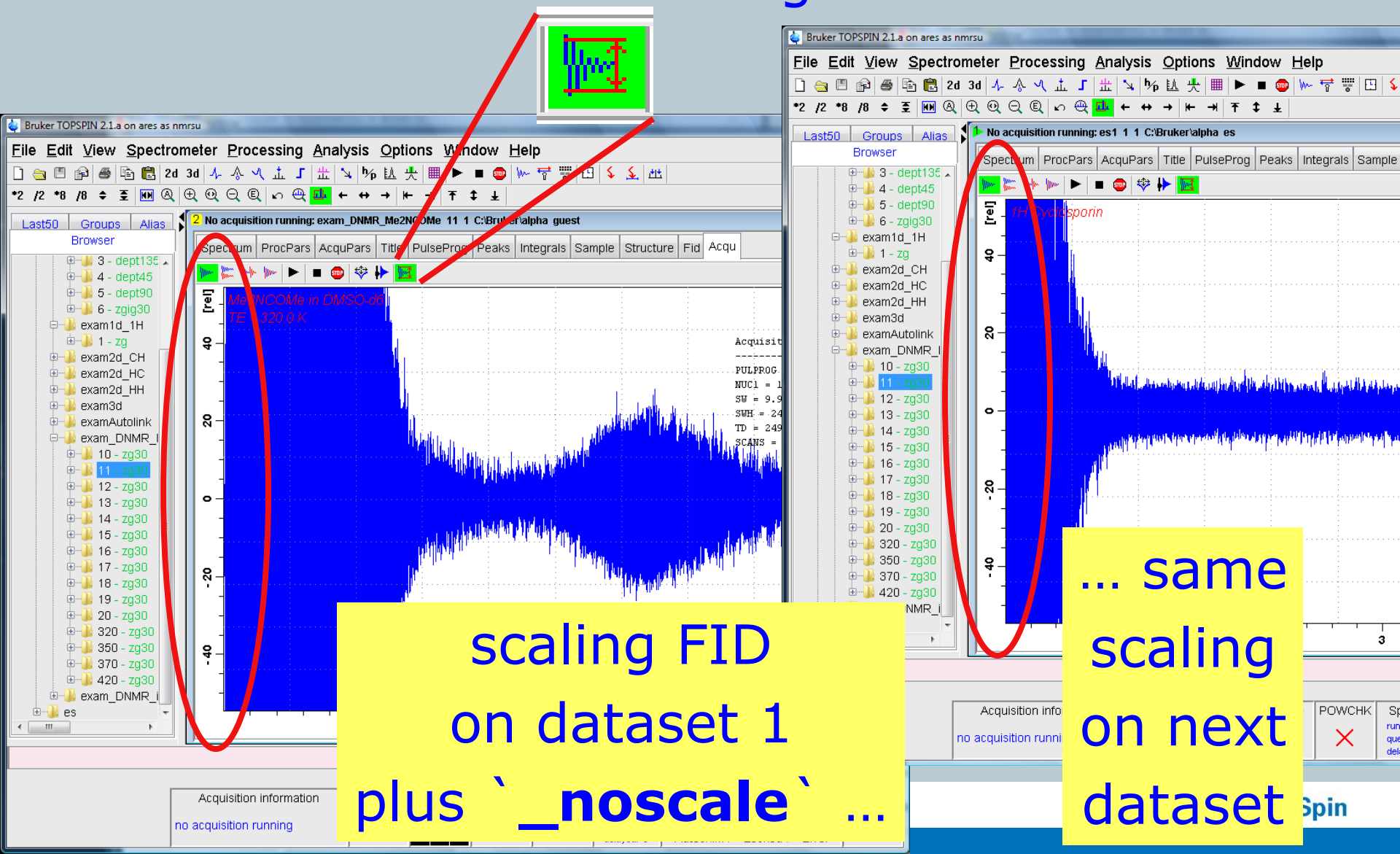
FID display

Default: Every FID is automatically scaled:



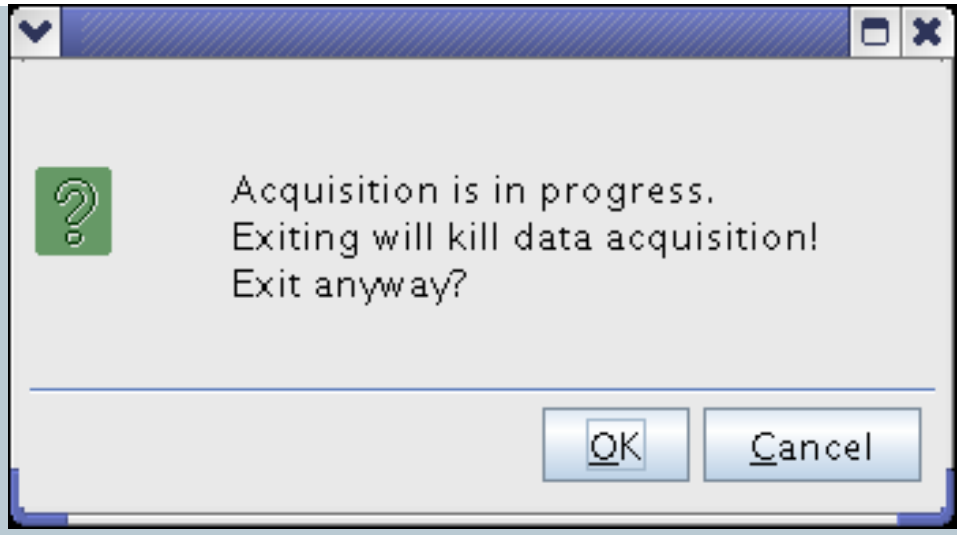
FID display

New feature: The FID scaling can be fixed:



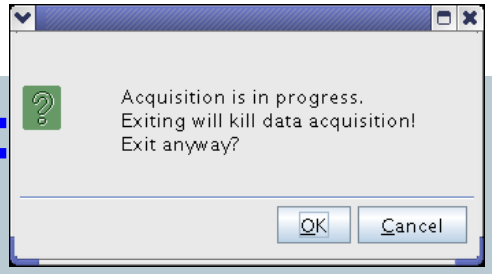
TopSpin exit messages

1. Acquisition is running:

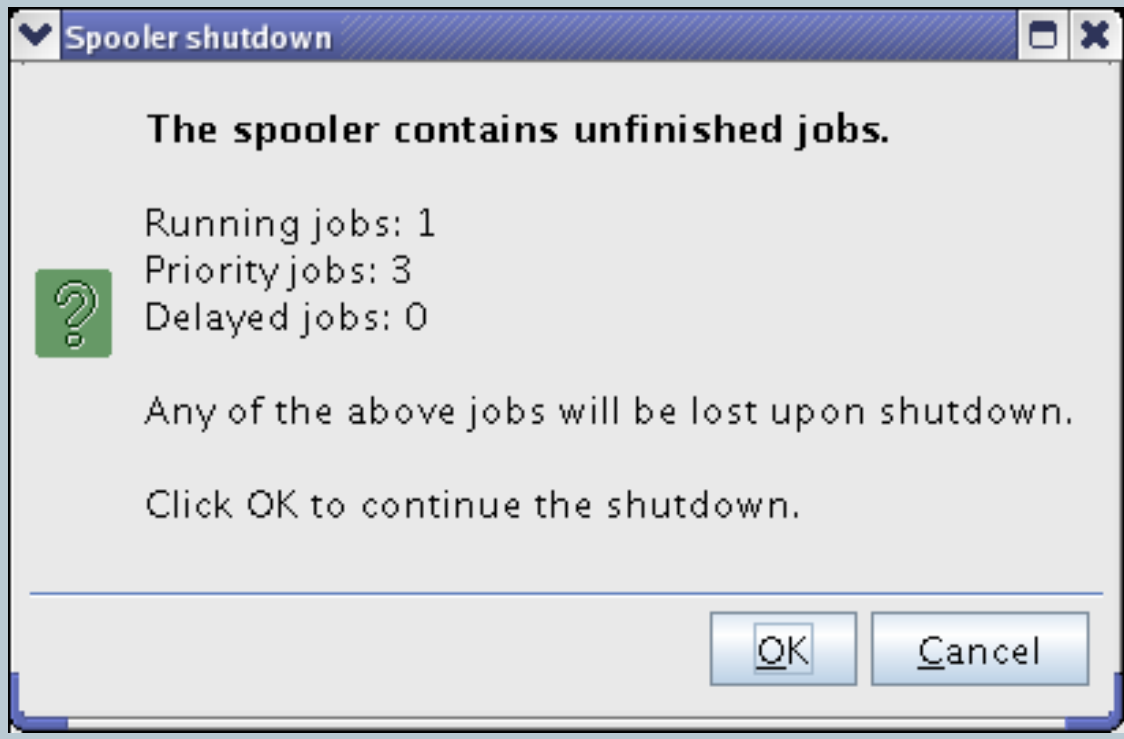


TopSpin exit messages

1. Acquisition is running:

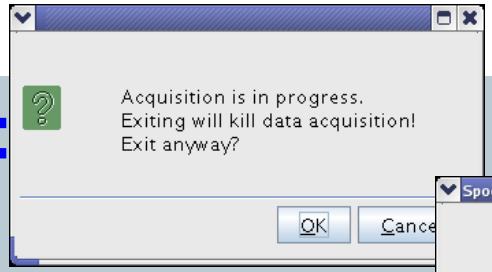


2. Spooler contains unfinished jobs:

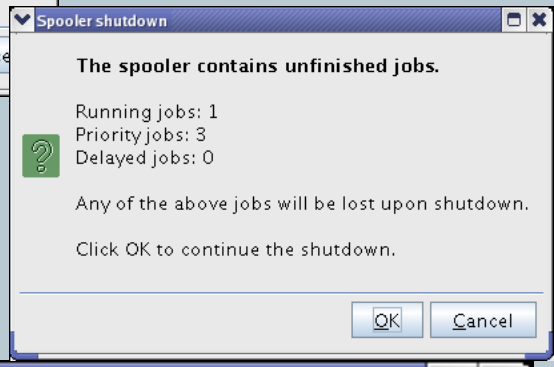


TopSpin exit messages

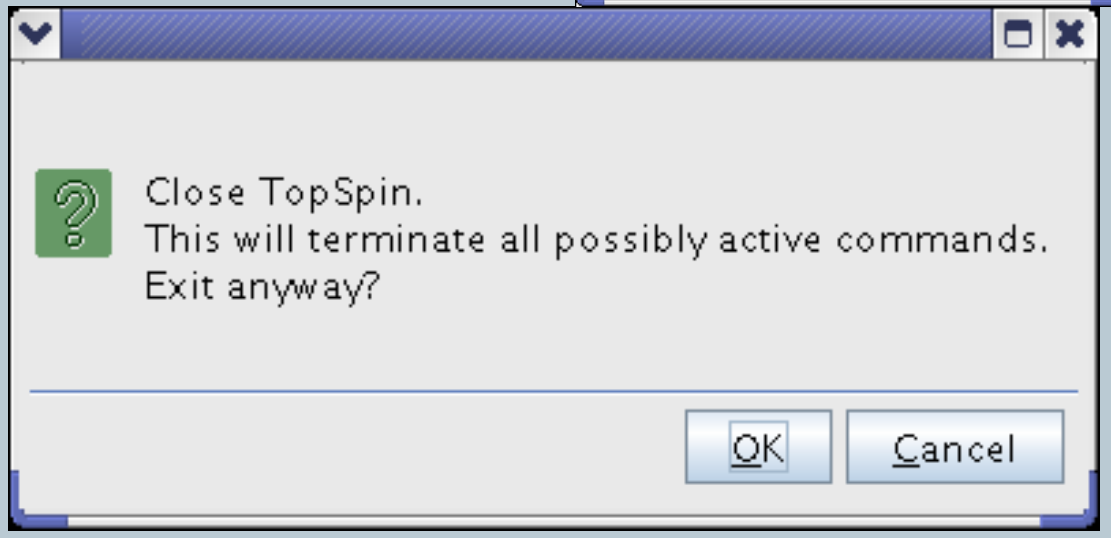
1. Acquisition is running:



2. Spooler contains unfinished jobs:

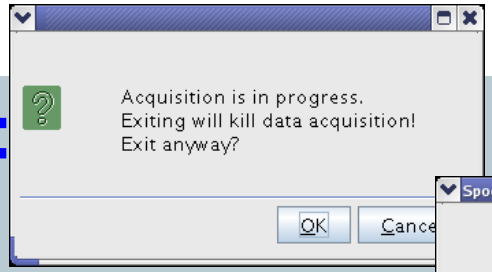


3. Default message:

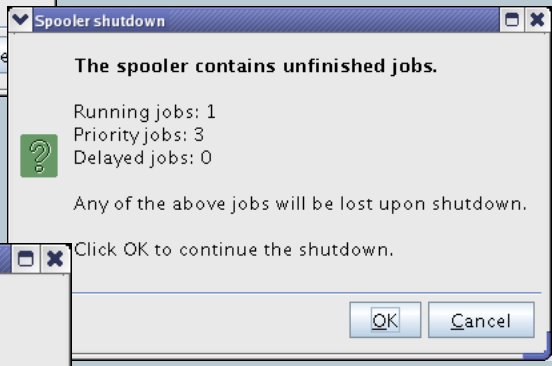


TopSpin exit messages

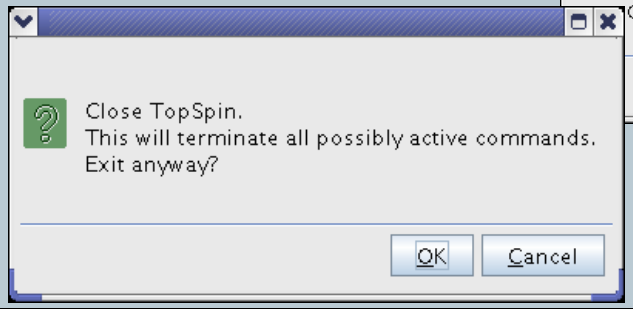
1. Acquisition is running:



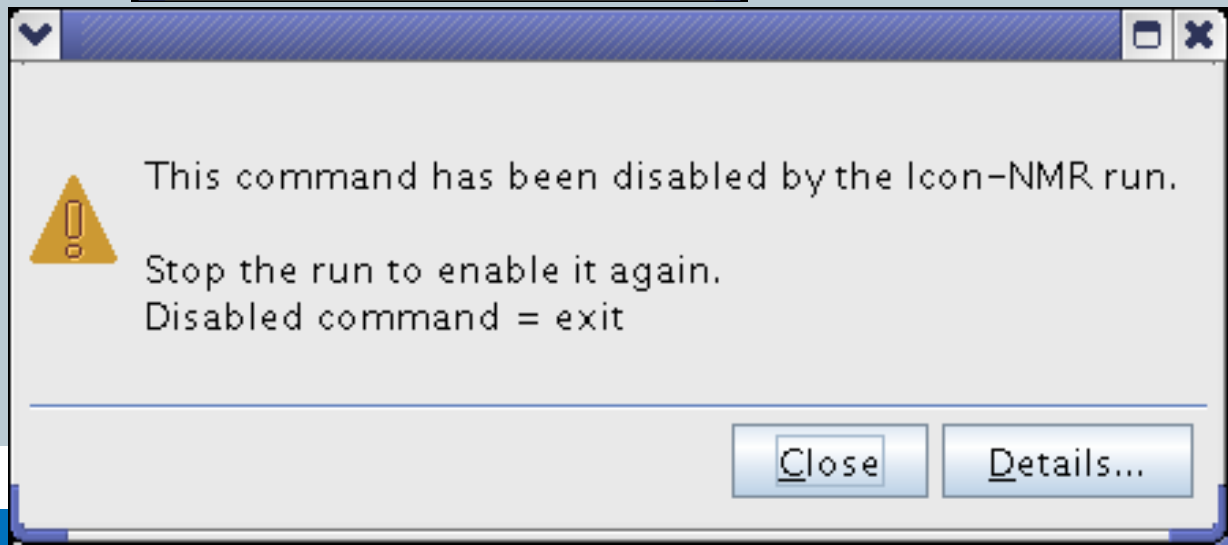
2. Spooler contains unfinished jobs:



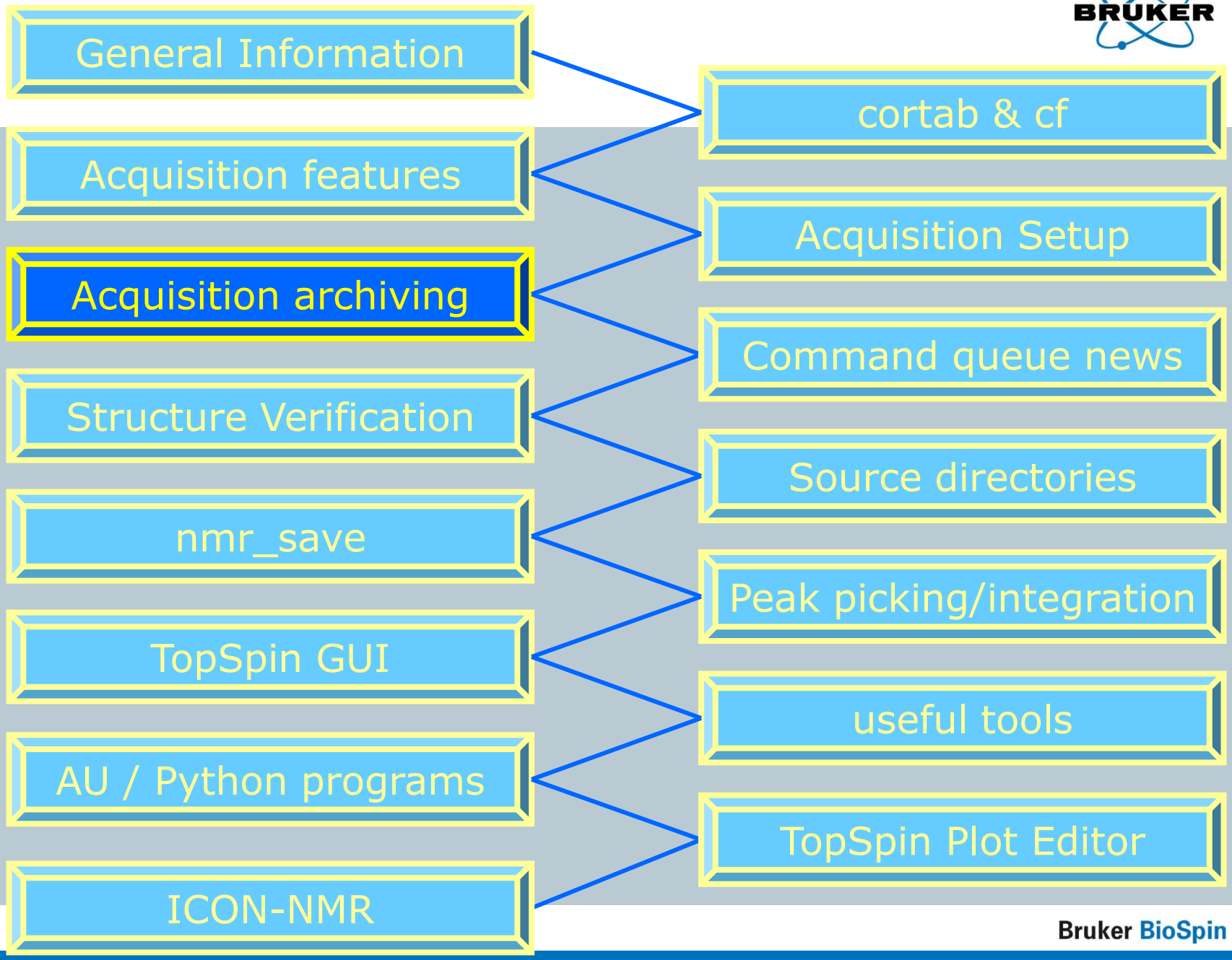
3. Default message:



4. No exit during an active ICON-NMR run:

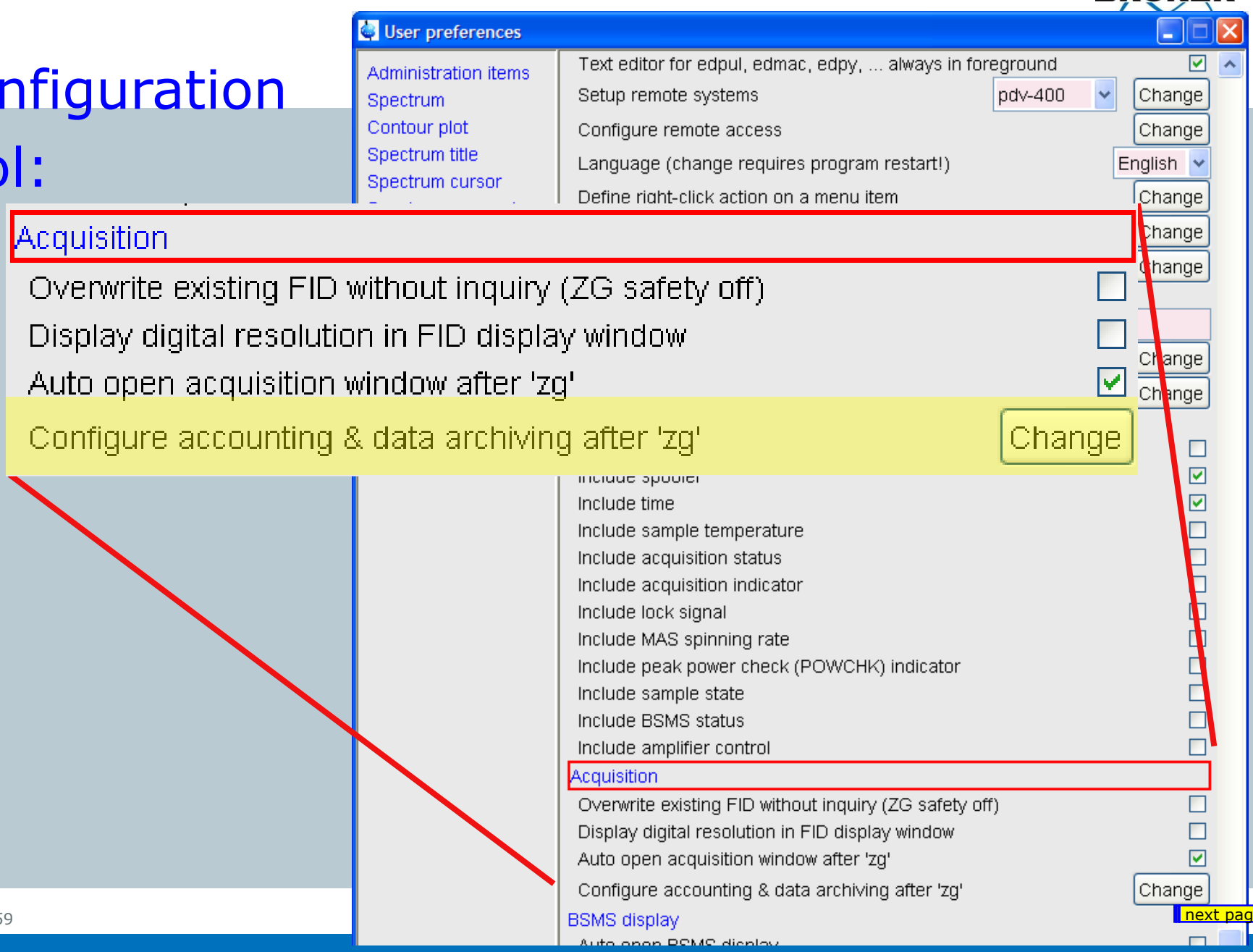


Content


General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

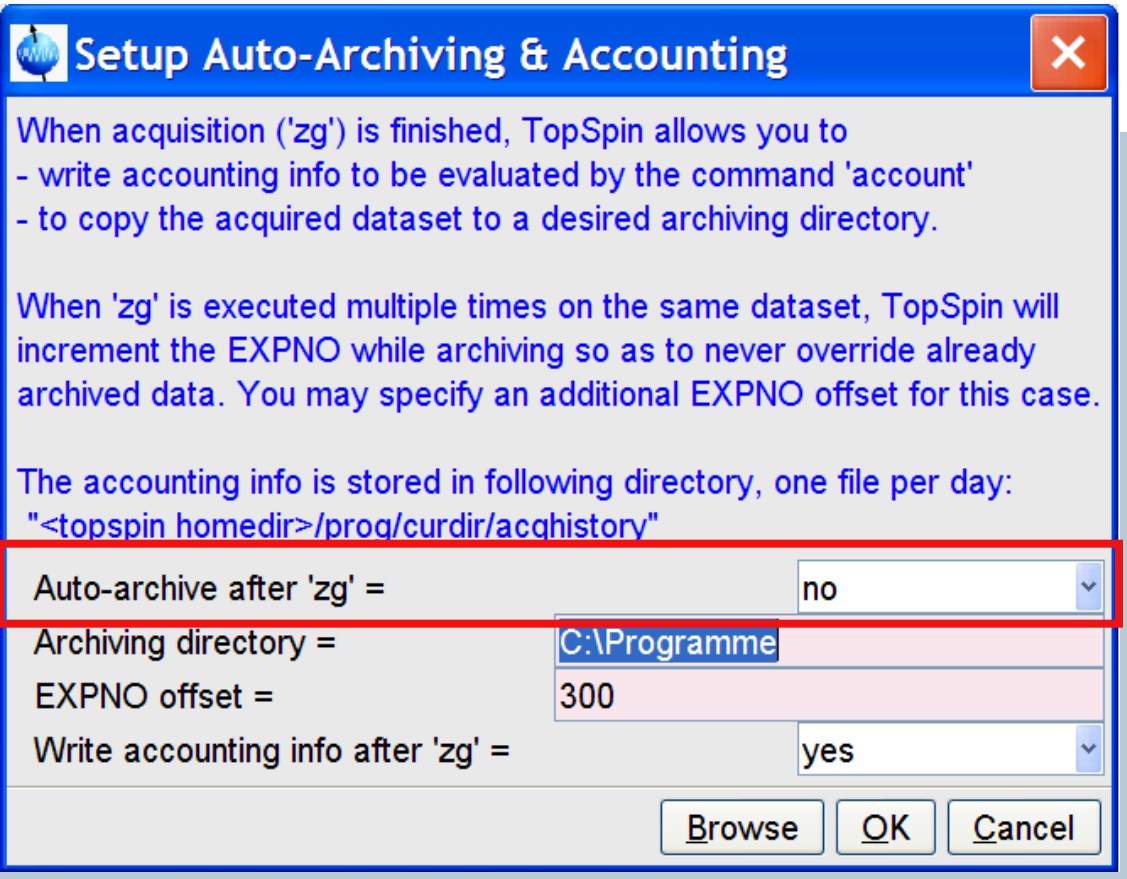
Archiving and accounting in TopSpin

Configuration tool:



next page

Archiving configuration



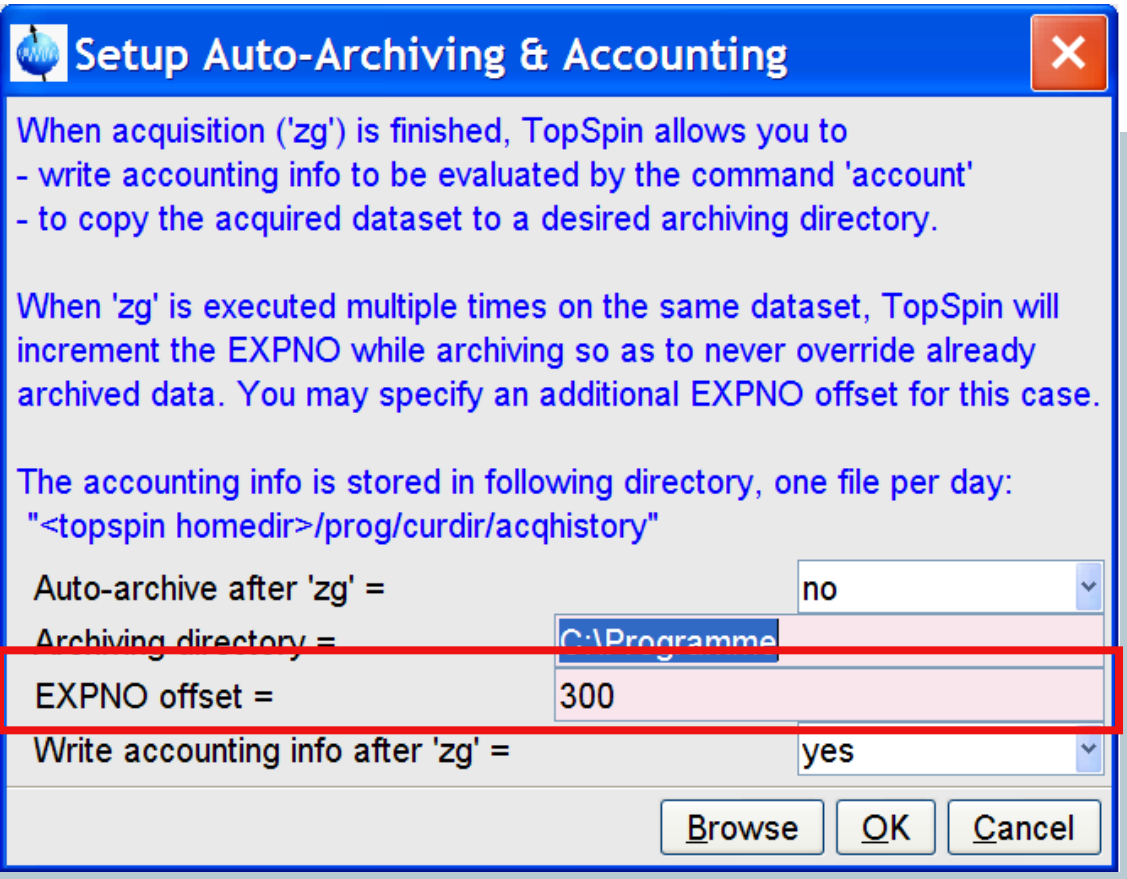
Like archive option in ICON-NMR

- will archive each acquisition which has been started from within TopSpin GUI

next page

(for AU programs: use '**XCMD("sendgui zg")**'

Archiving configuration

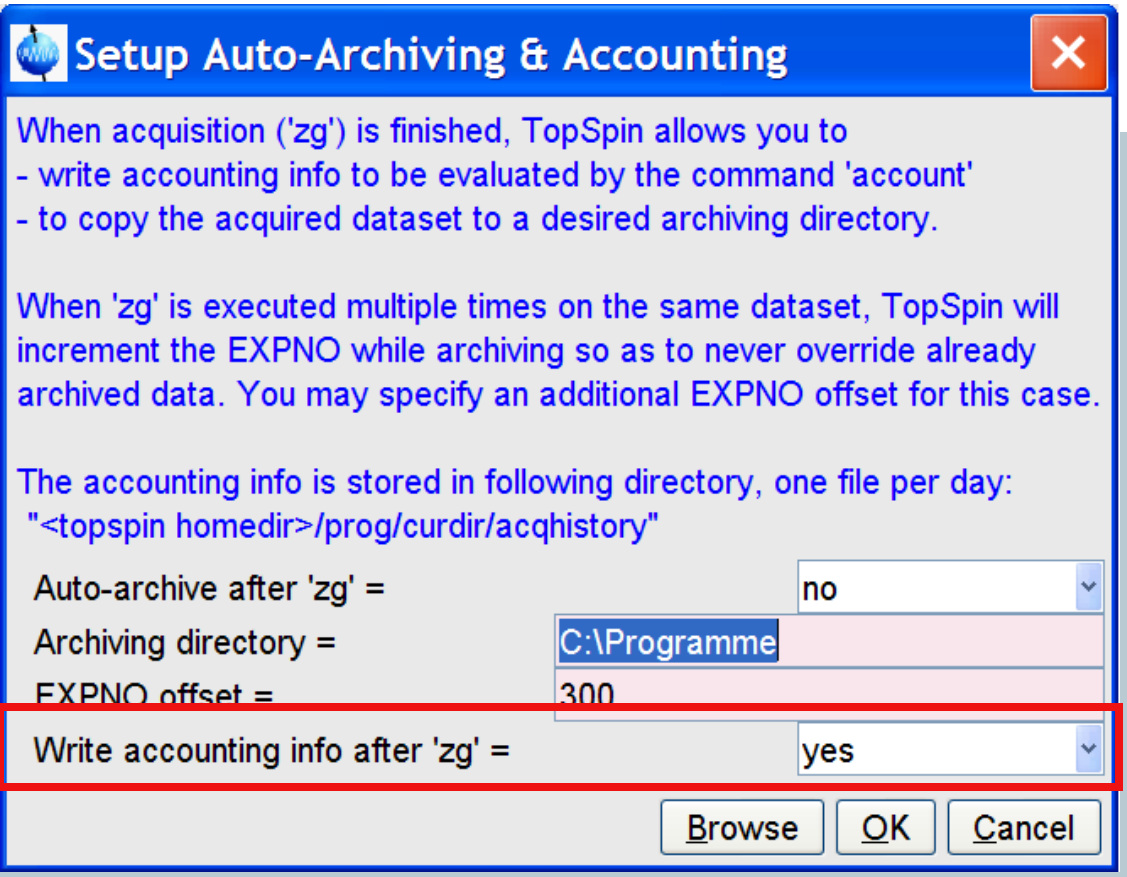


If an experiment is executed second time

- dataset in the archive can be overwritten or a new expno can be added. Increment is user-specific.

next page

Accounting configuration



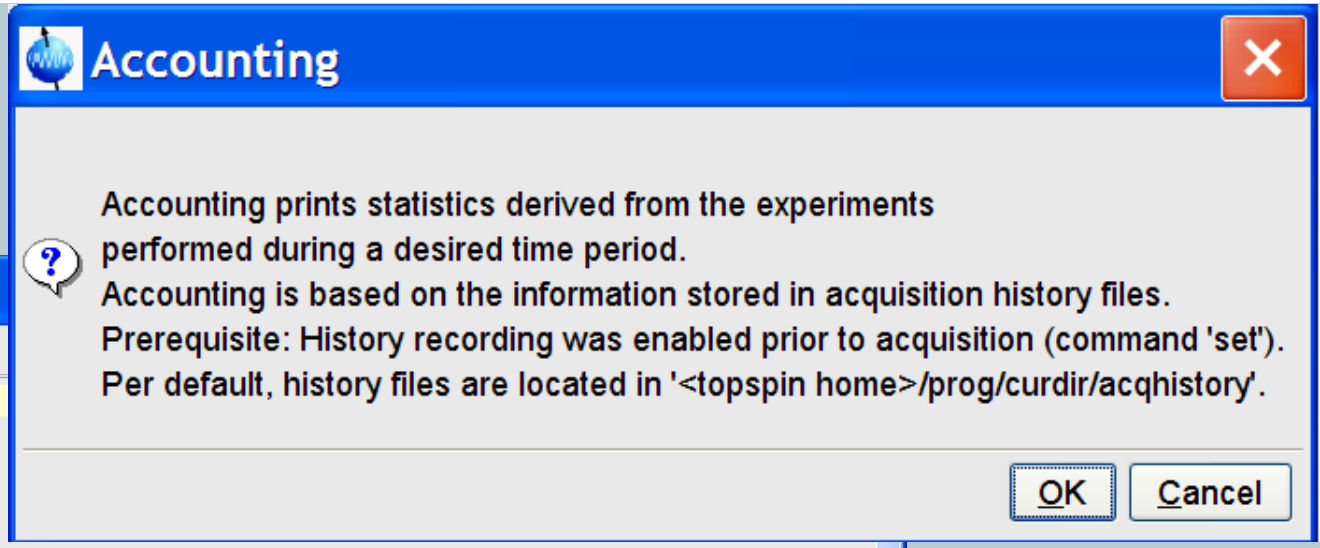
New command **account** is implemented

that checks the acquisition history file.

next page

Accounting

New TopSpin command **account** :

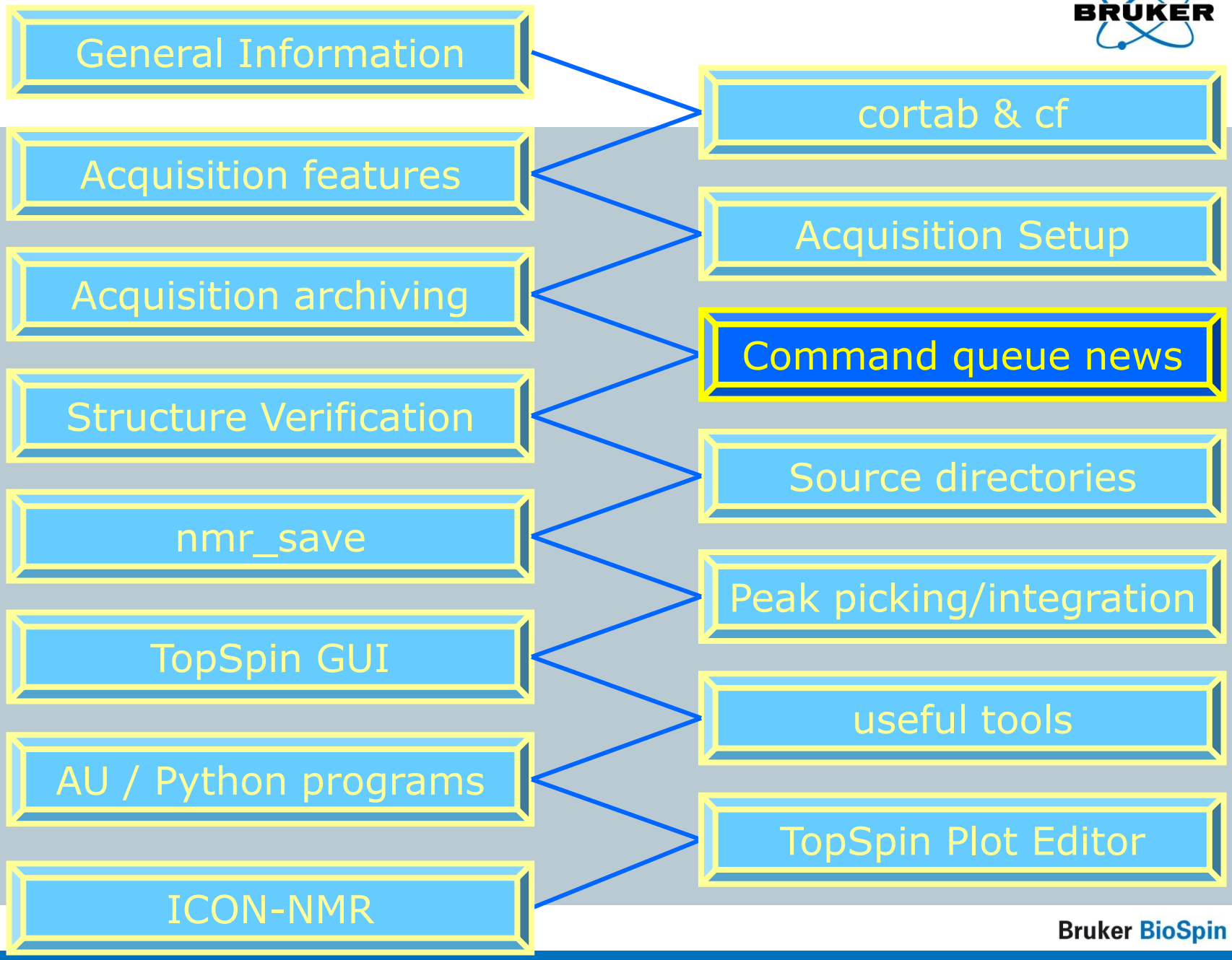


Accounting Protocol

File Edit Search

```
1  Accounting Protocol
2  Created: 2007-02-16 09:49:39 CET
3  TopSpin: 2.1.a
4
5  User: bg
6  #Datasets    Dim      Exp.Time    Failed
7        3       1        3.55 sec       1
8        6       2       21.86 sec       0
9        5      >2        7.08 sec       0
10 Sum =
11      14     Any       32.49 sec       1
12
13
14 Period
15 From: 2007-01-31 14:49:47 CET
16 To:   2007-02-02 10:44:57 CET
17
18 The following datasets had "acquisition failed" status:
19
20 c:\bruker\topspin\data\guest\nmr\exam1d_13C\1\pdata\1
21   failed xxx
22
23 ------------------------------------------------------------
24
25
```

Content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TopSpin Plot Editor

Command spooler

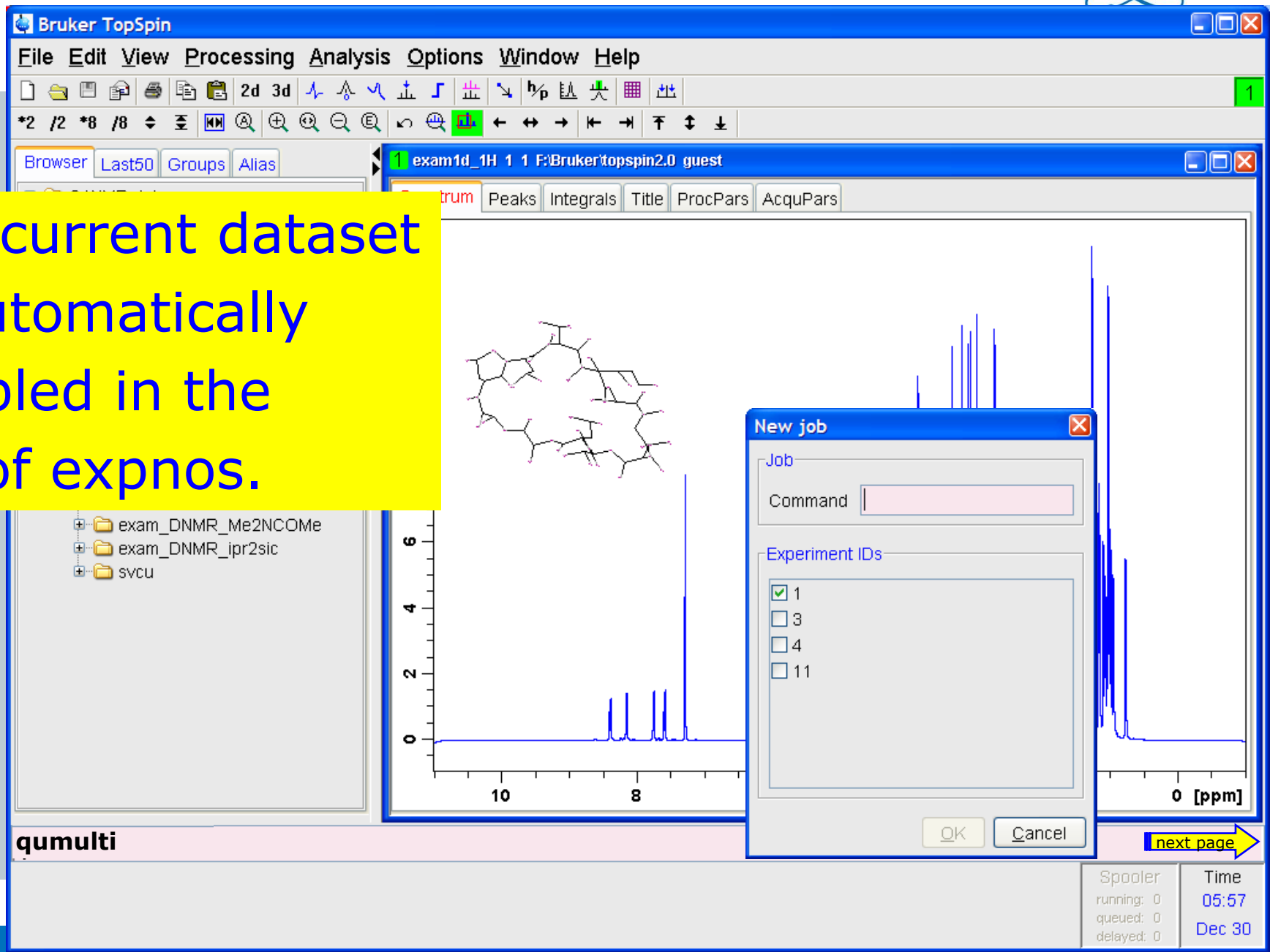
It is now possible to define the experiment number on which a command should be queued:

qumulti

atmulti

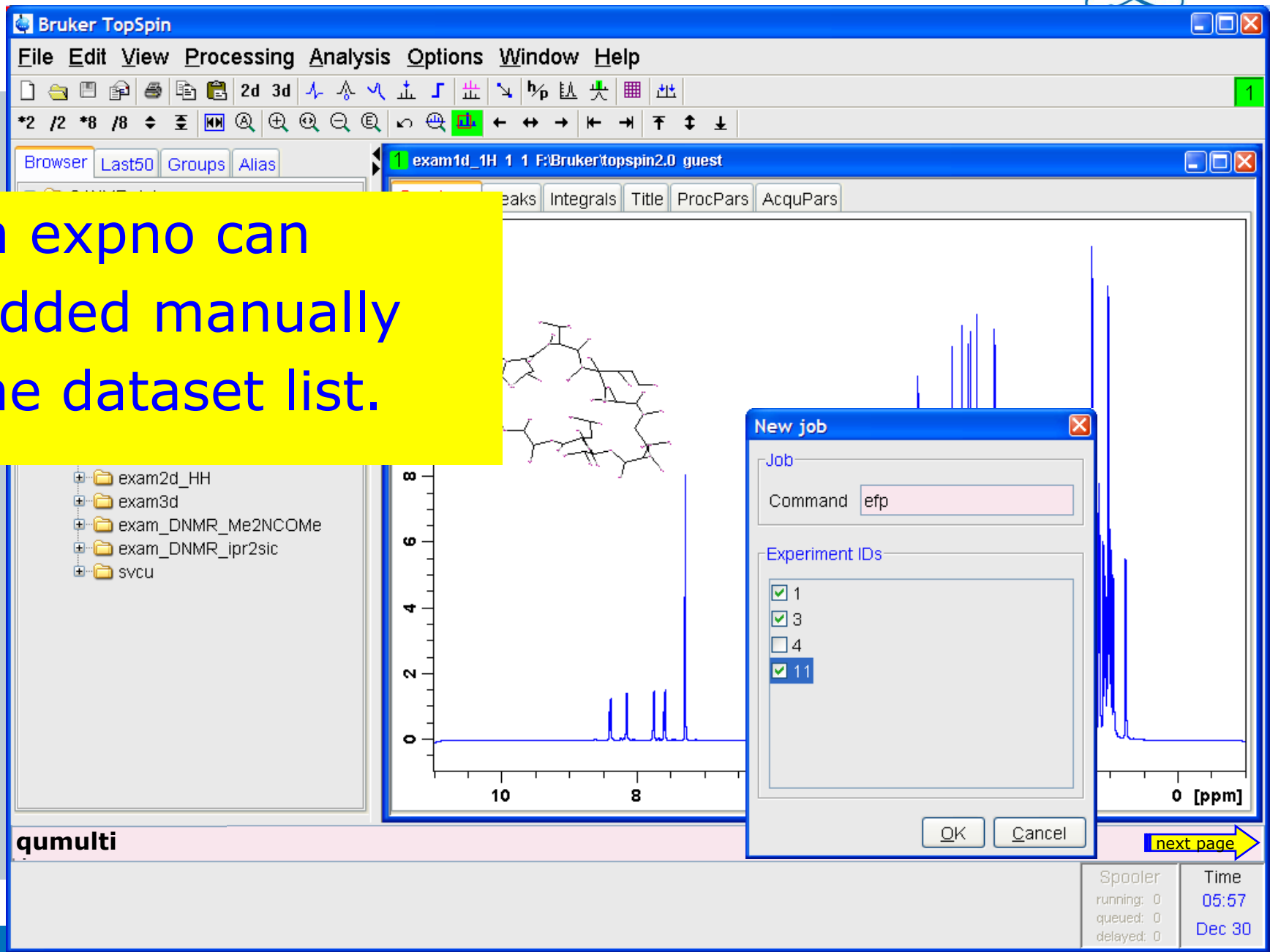
next page

qumulti



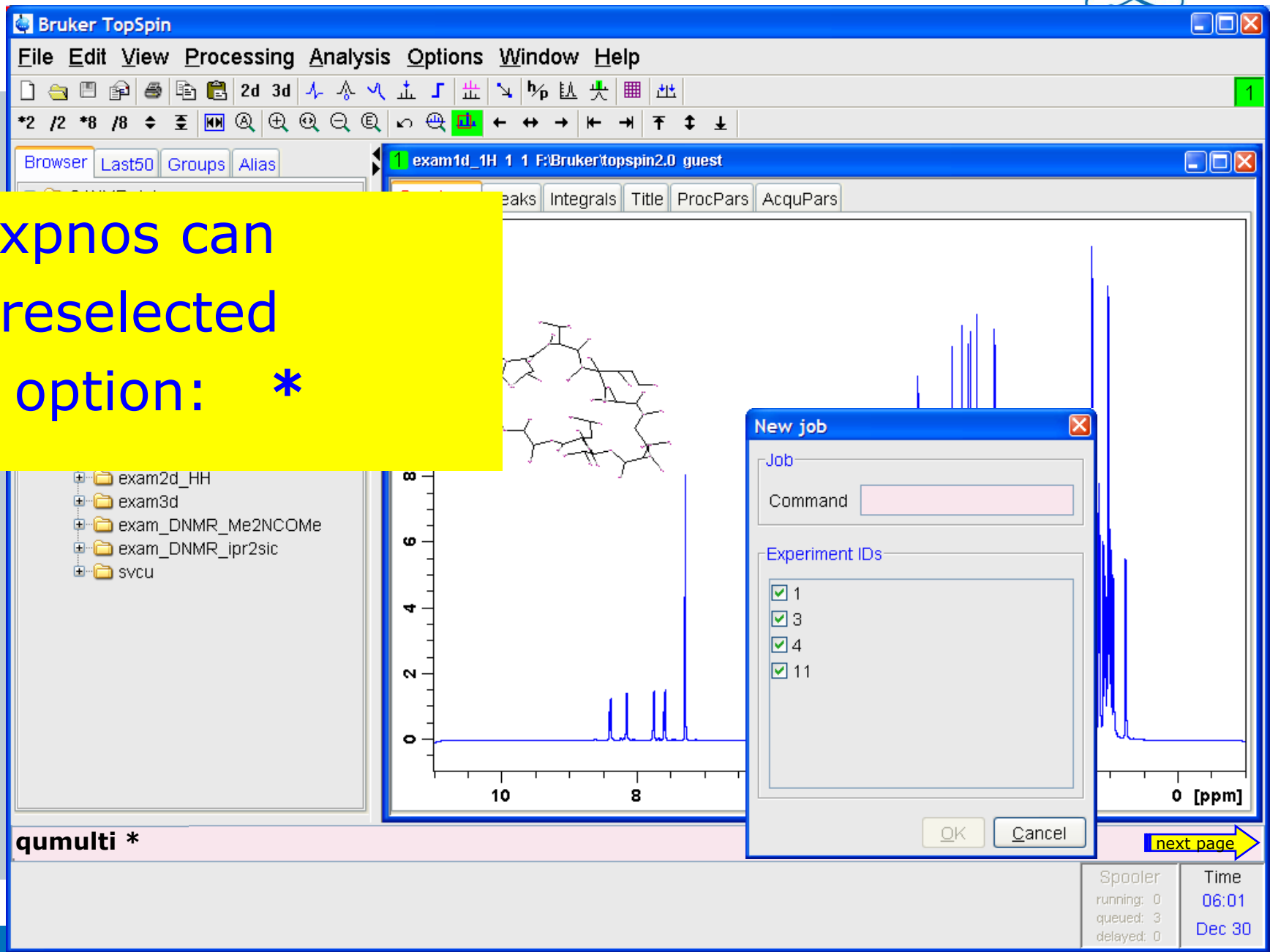
The current dataset is automatically enabled in the list of expnos.

qumulti



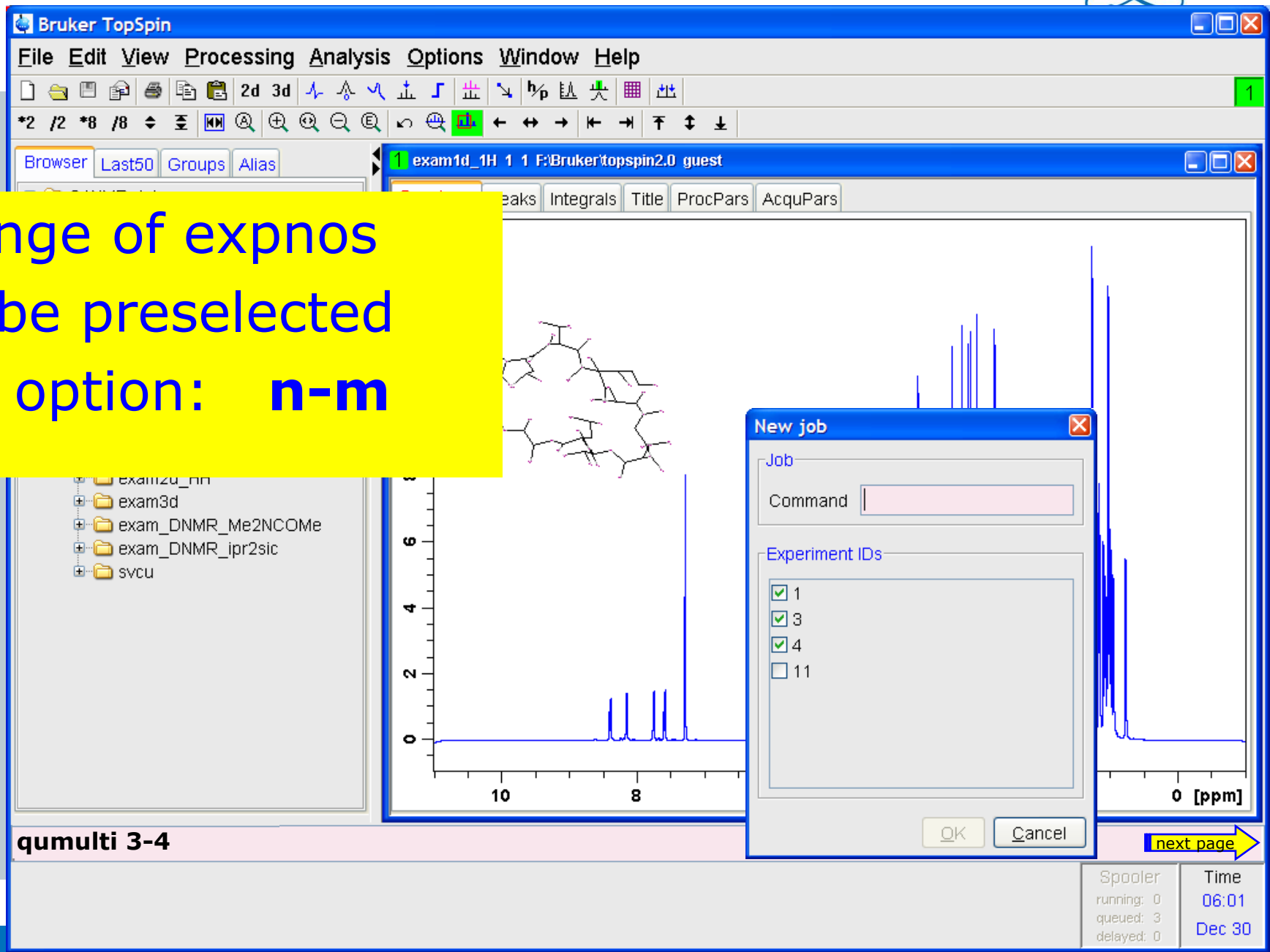
Each expno can be added manually to the dataset list.

qumulti *



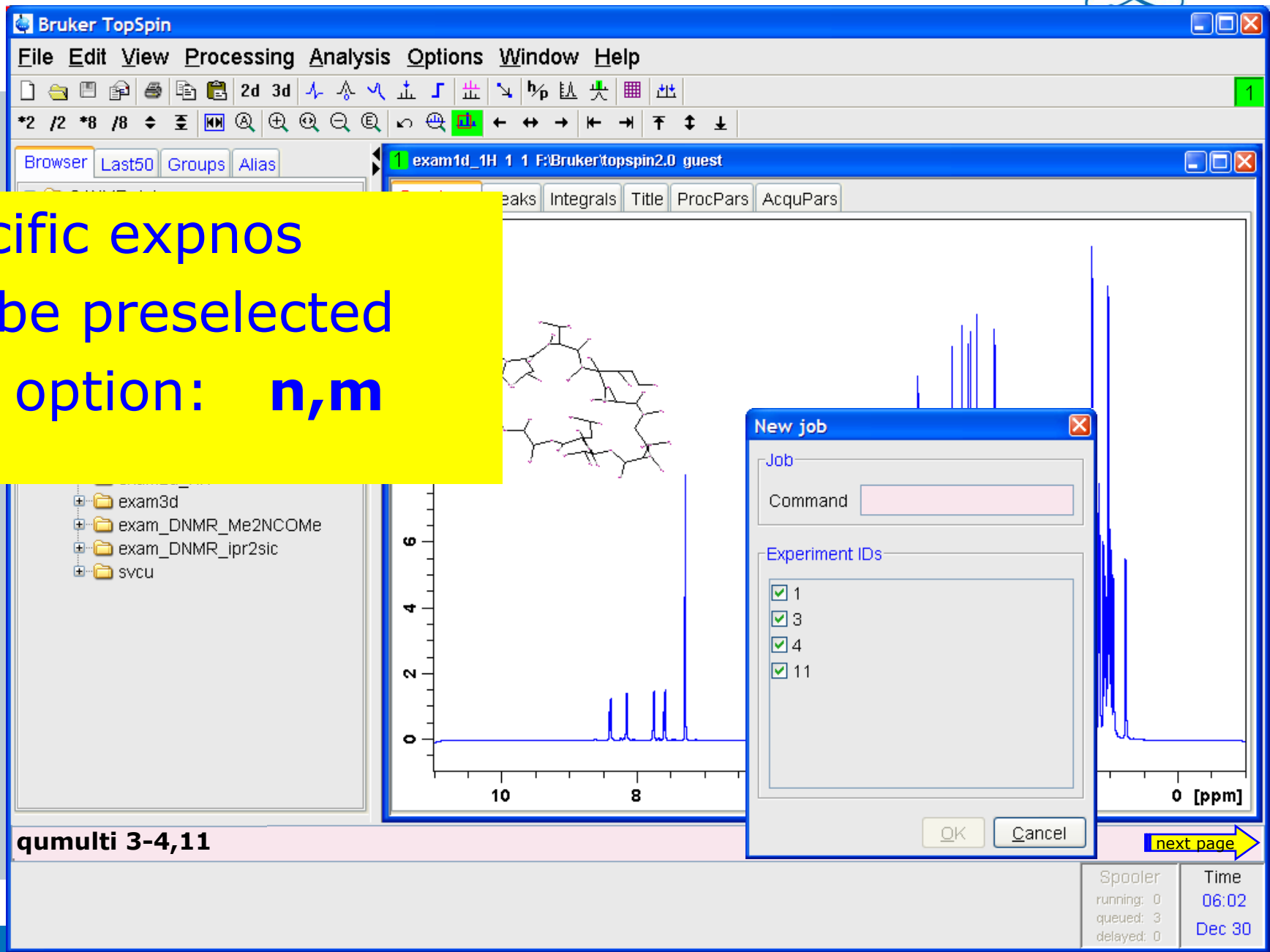
All expnos can be preselected with option: *

qumulti n-m



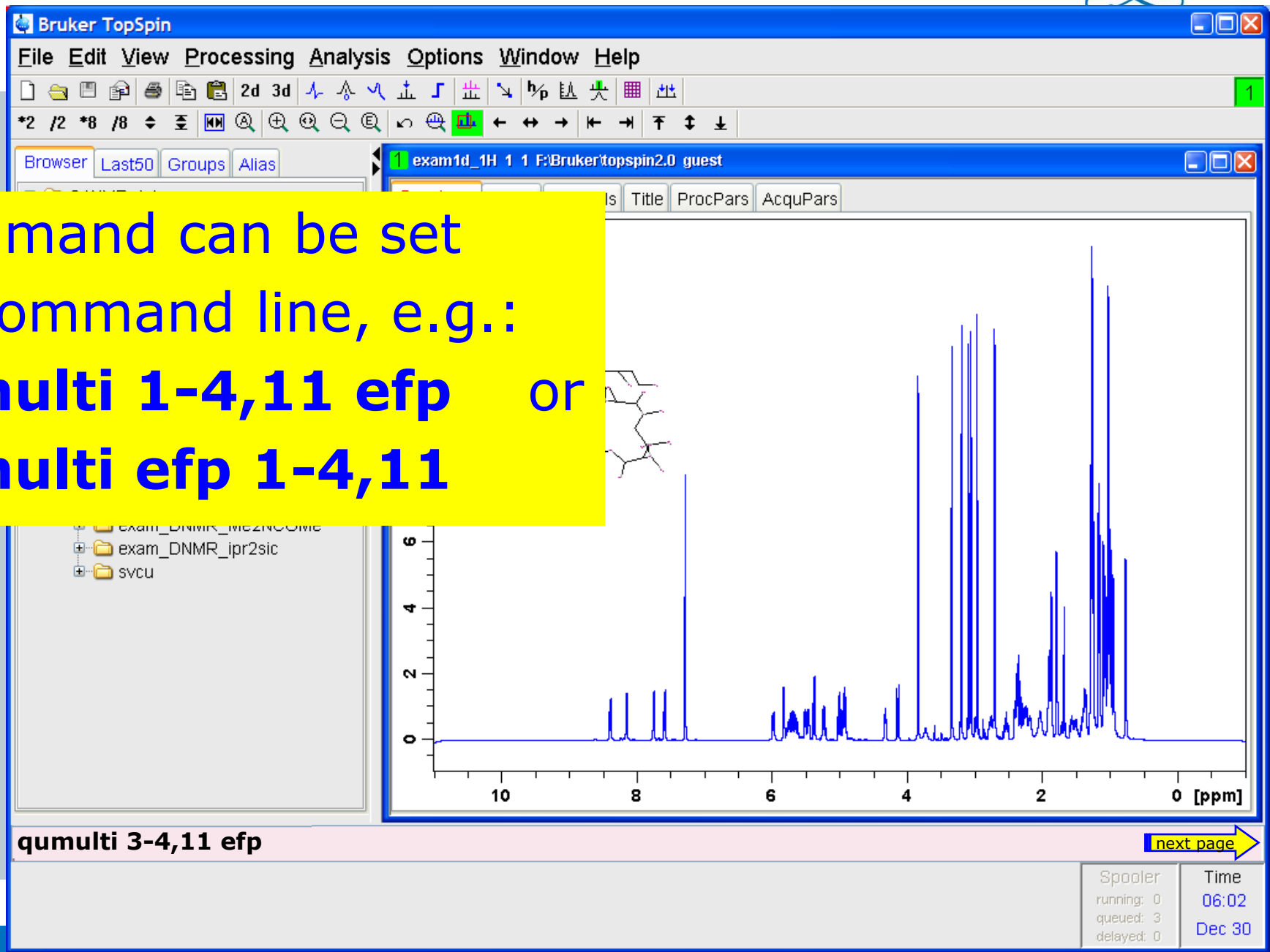
A range of expnos can be preselected with option: **n-m**

qumulti



Specific expnos
can be preselected
with option: **n,m**

qumulti



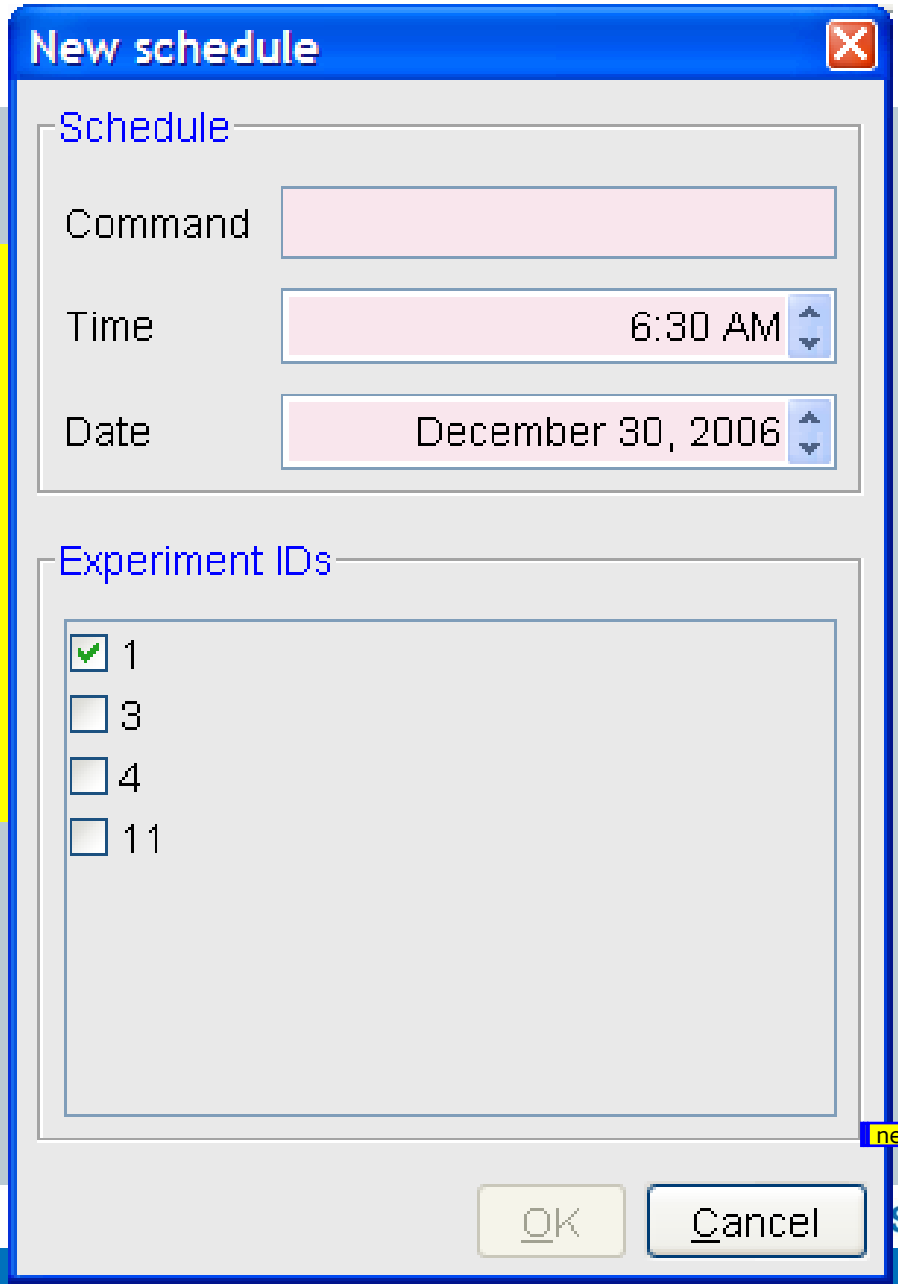
Command can be set on command line, e.g.:

qumulti 1-4,11 efp or

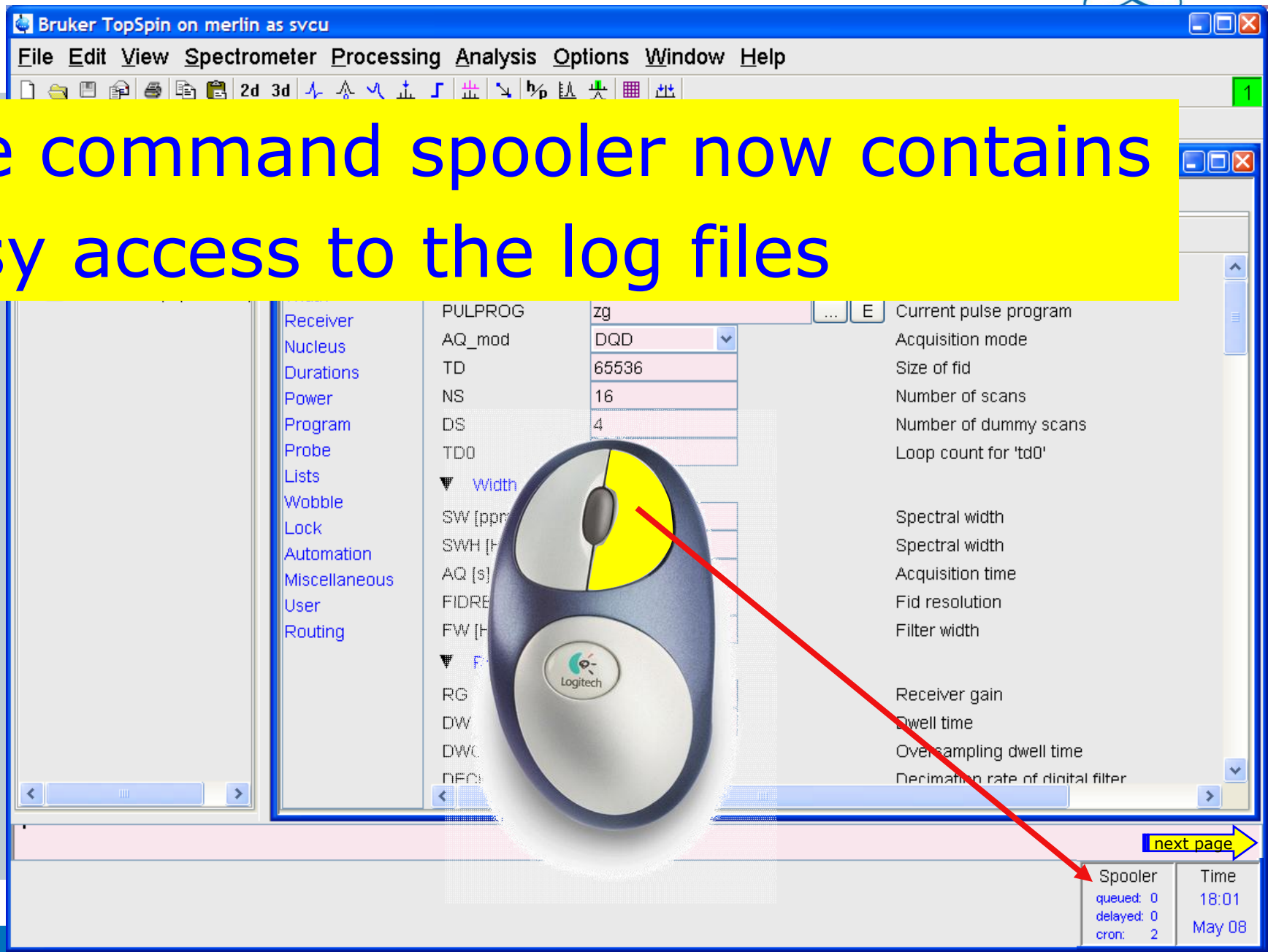
qumulti efp 1-4,11

atmulti

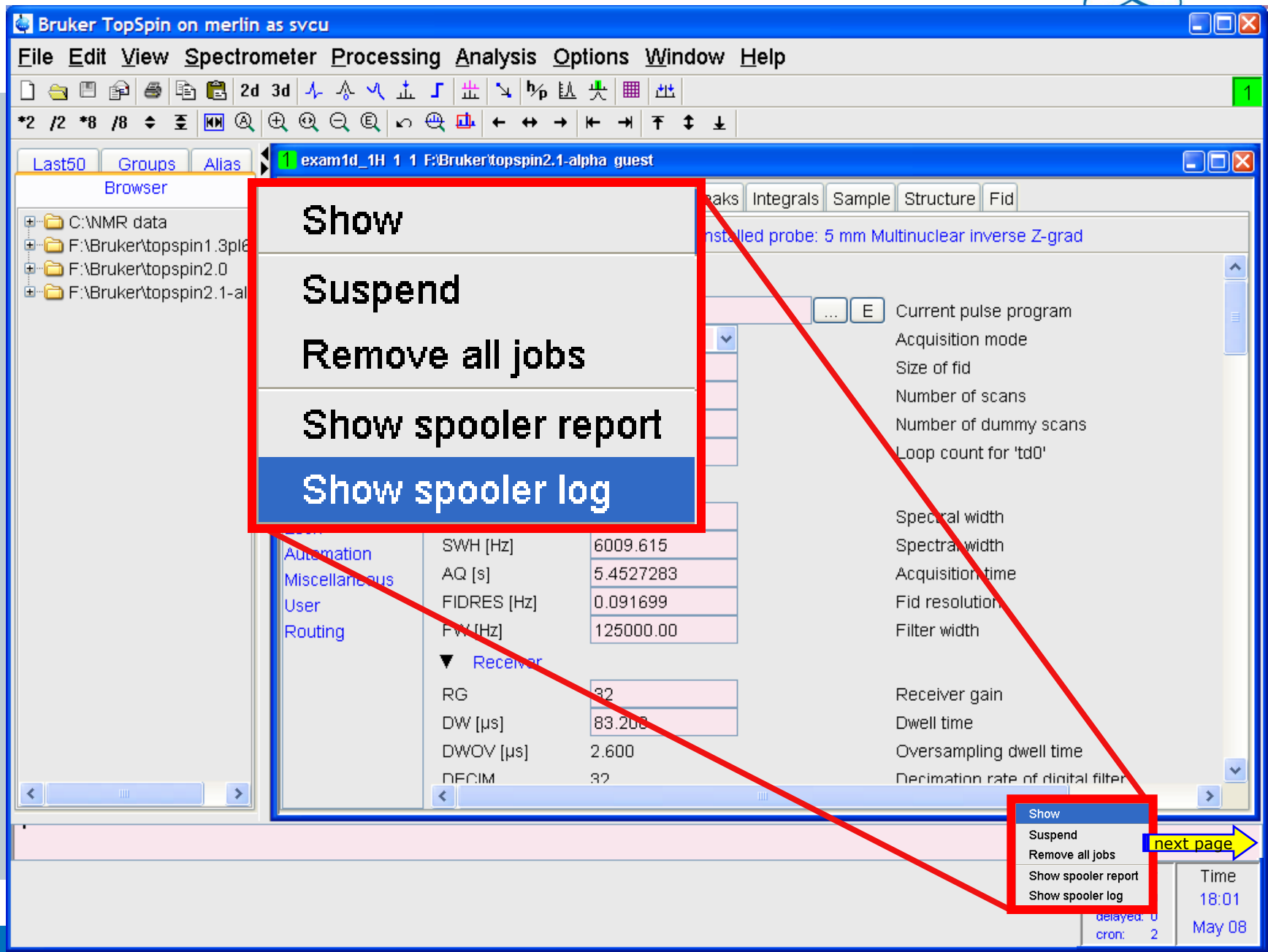
Same functionalities are available for the list of delayed jobs with command: **atmulti**



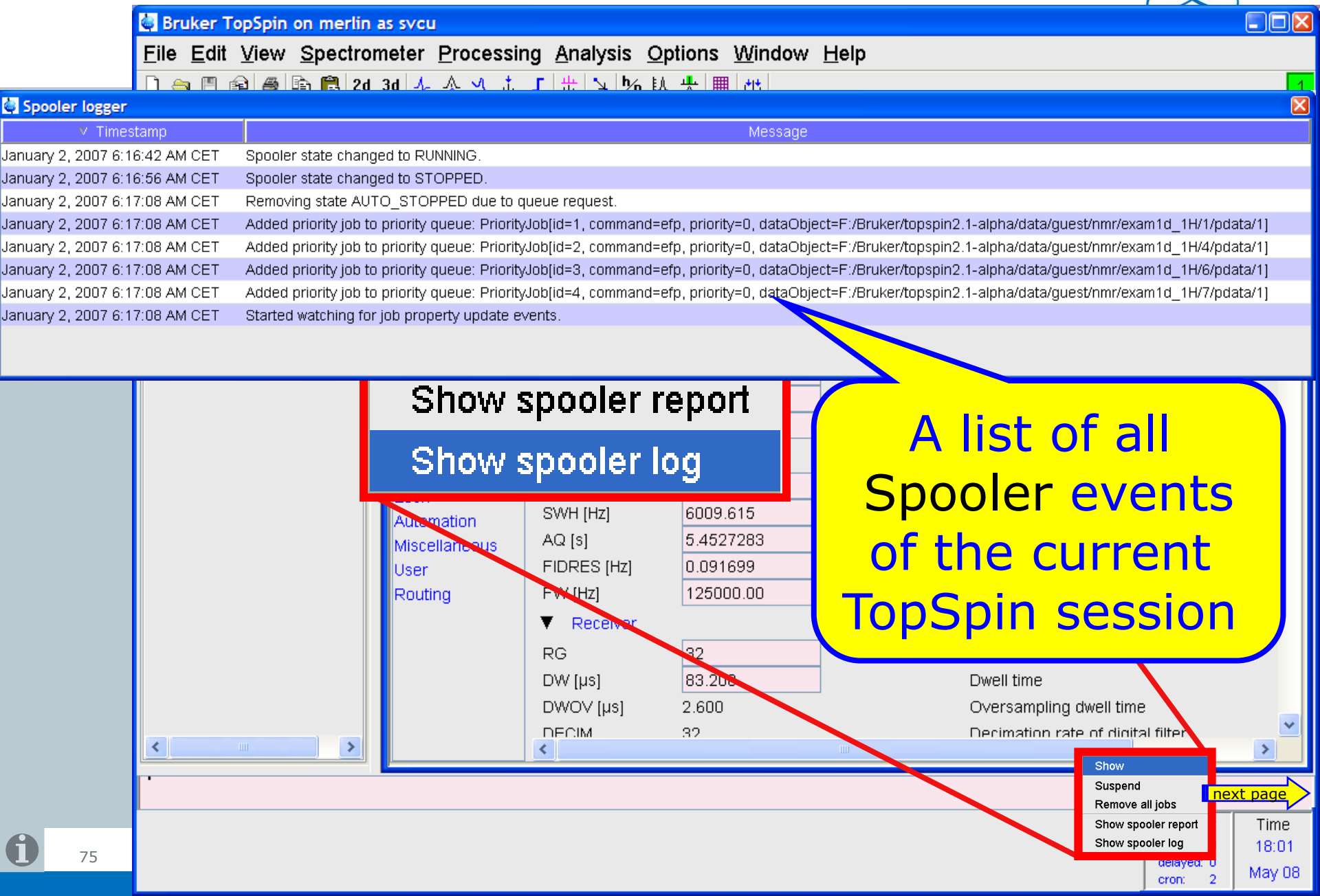
Command queue log file



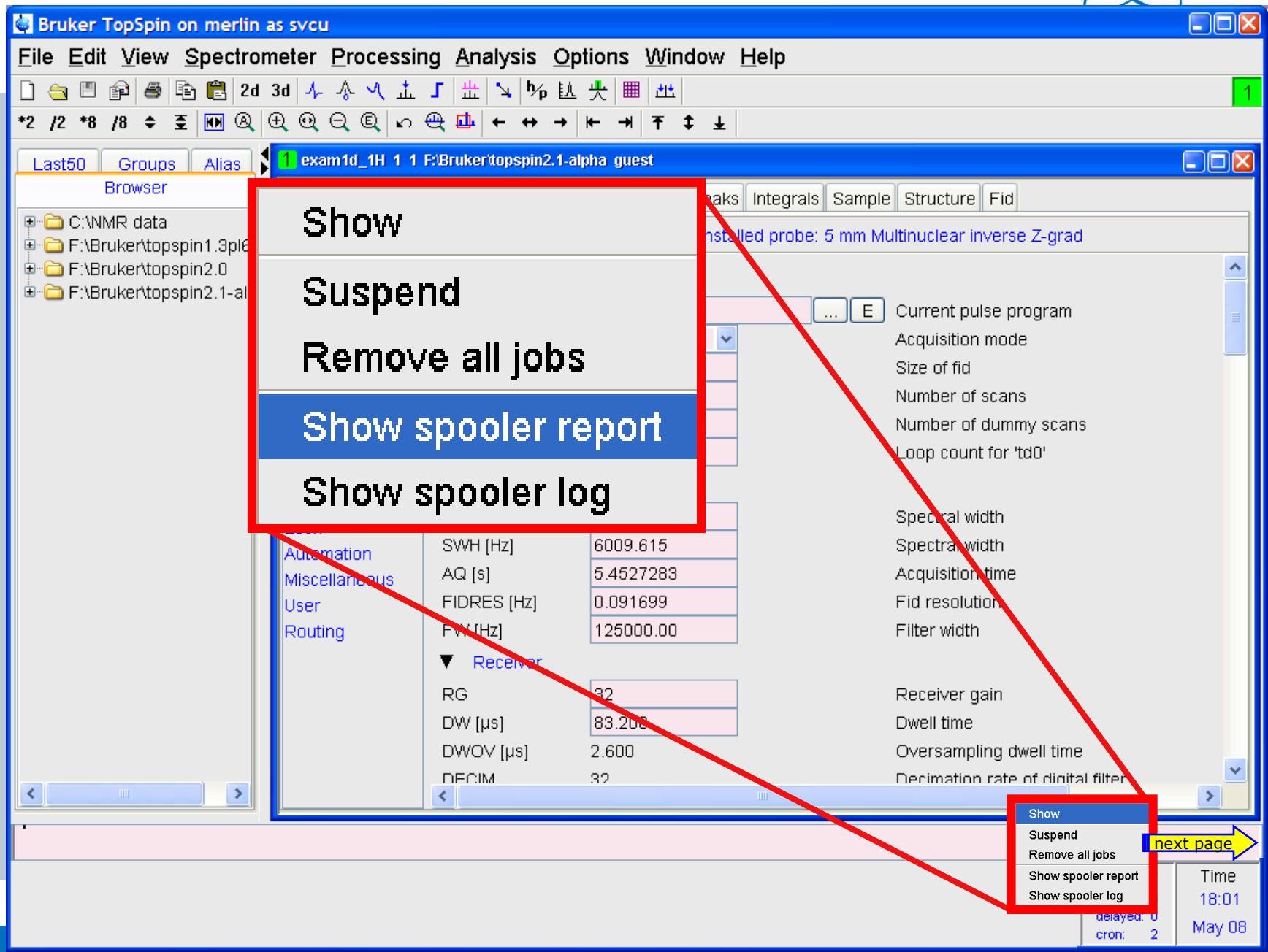
Command queue log file



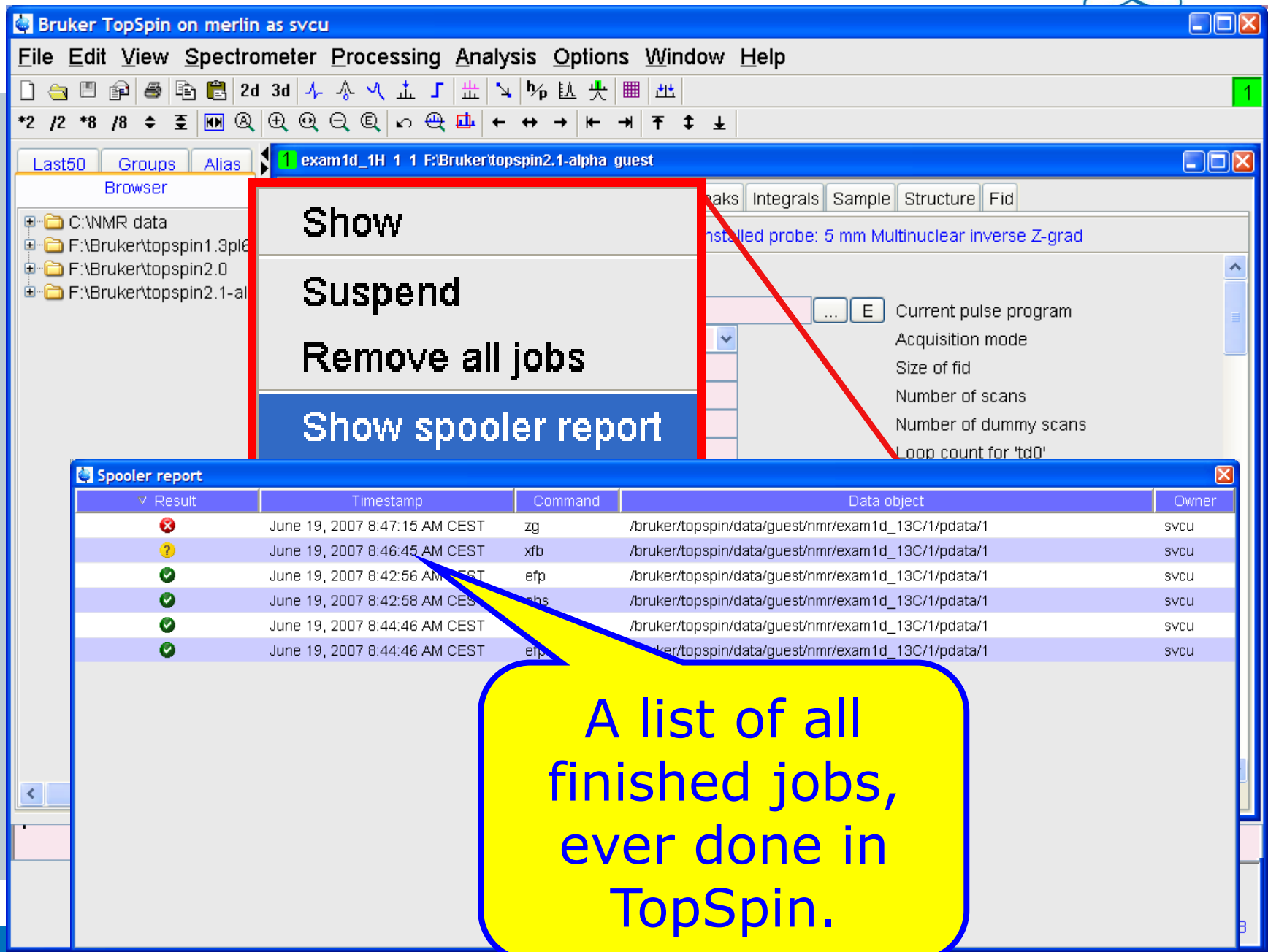
Command queue log file



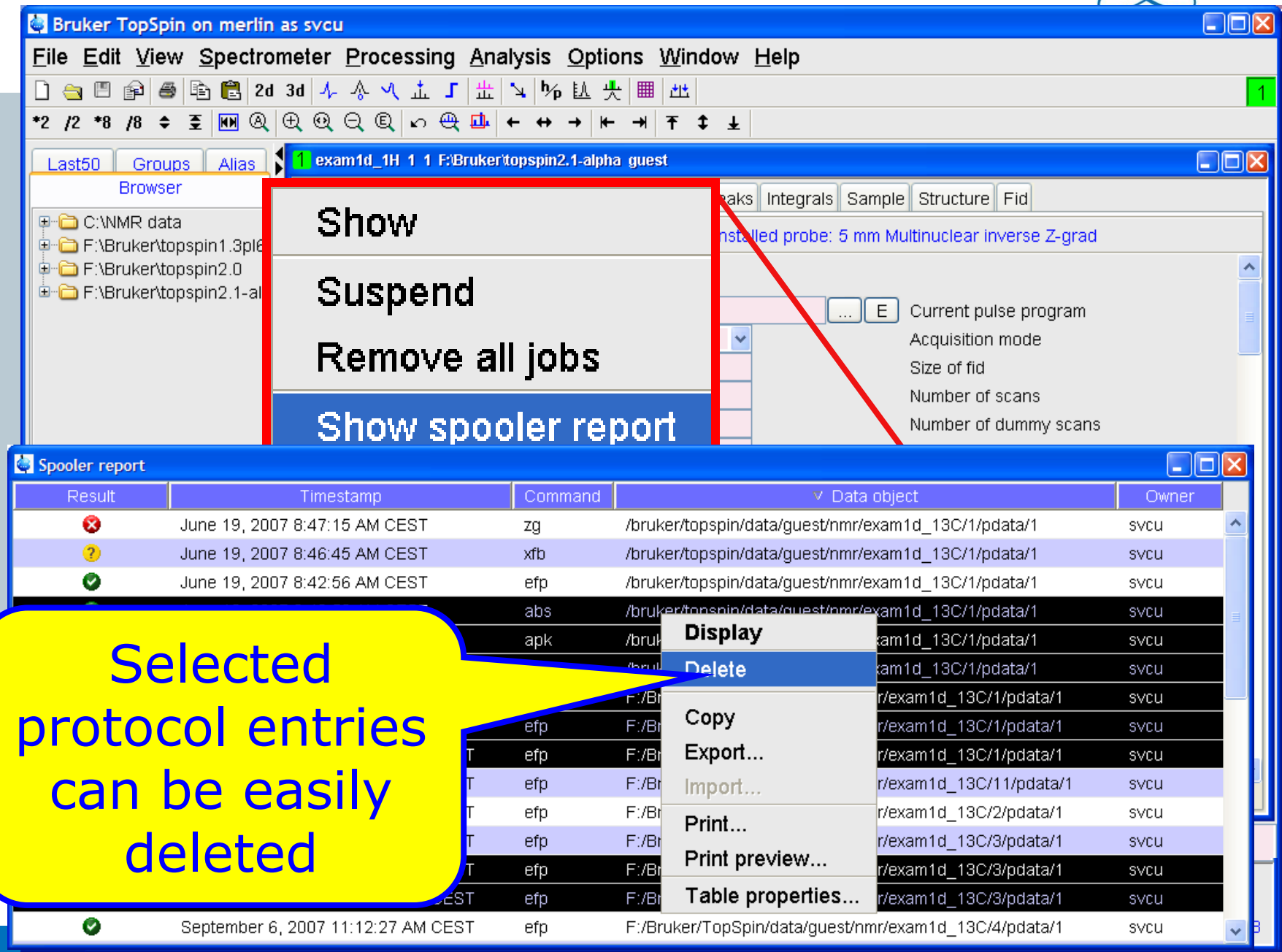
Command queue report file



Command queue report file

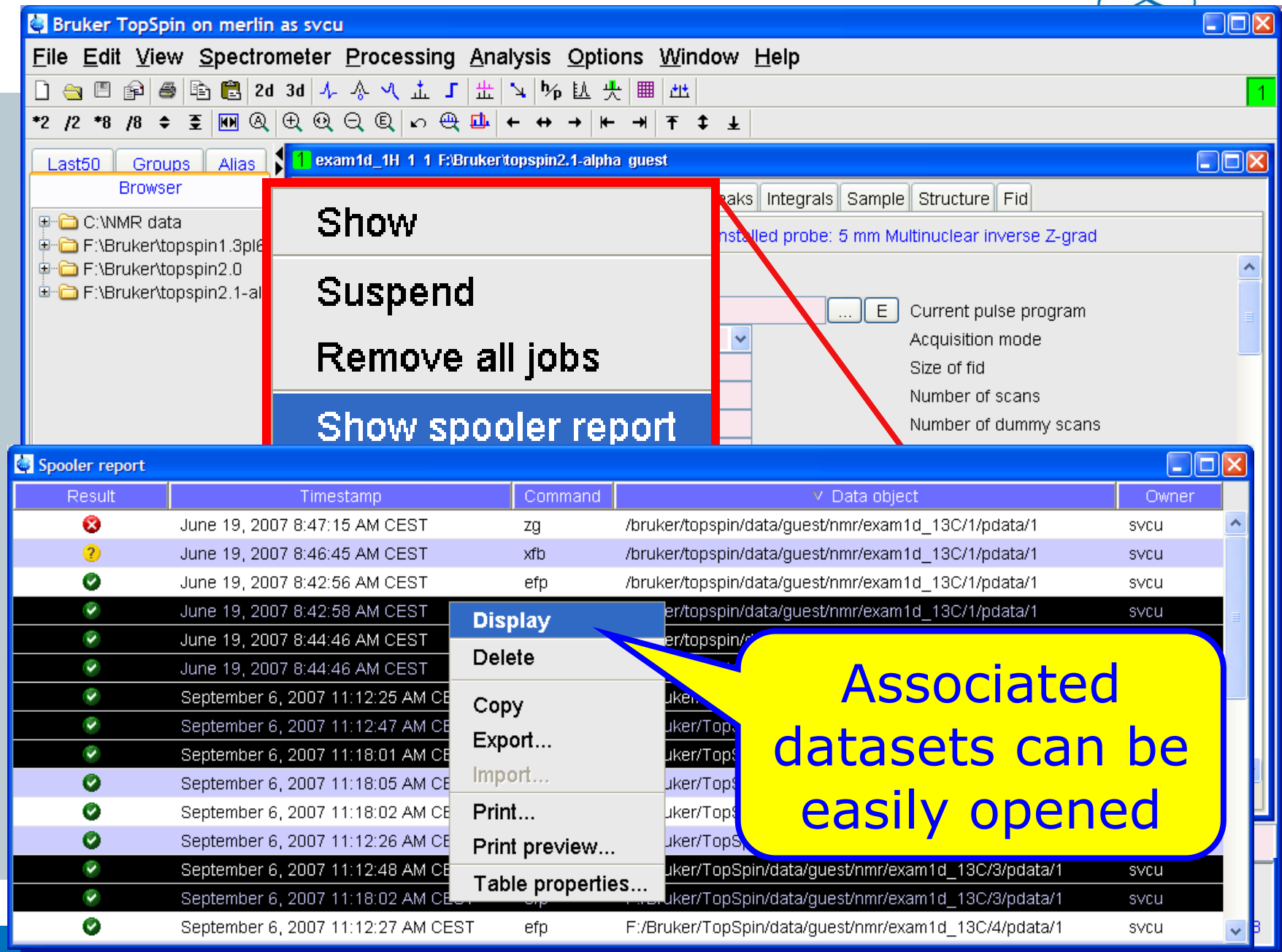


Command queue report file



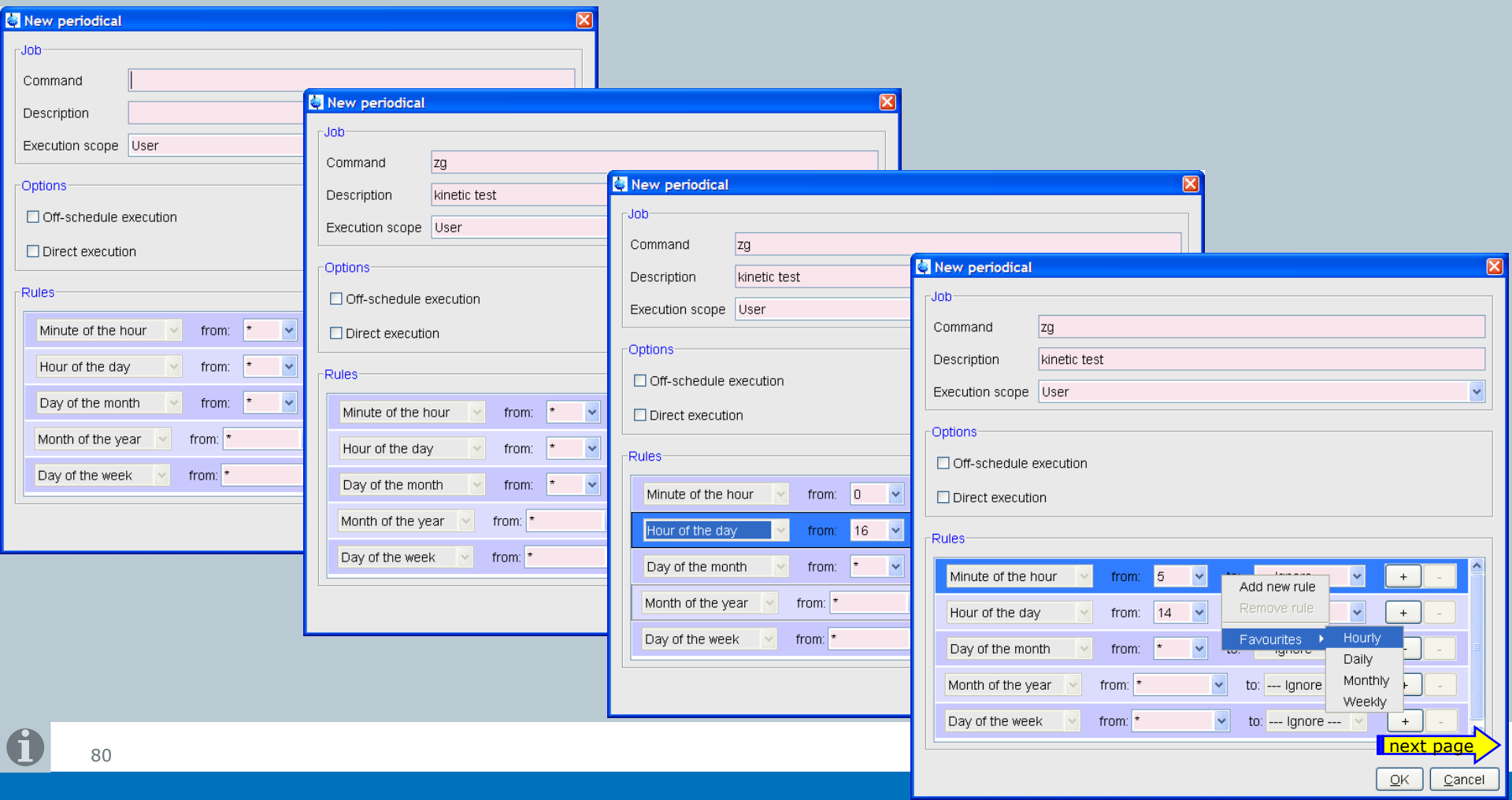
Selected protocol entries can be easily deleted

Command queue report file



New command: **cron**

cron allows executing a TopSpin command periodically at a specific time/date:

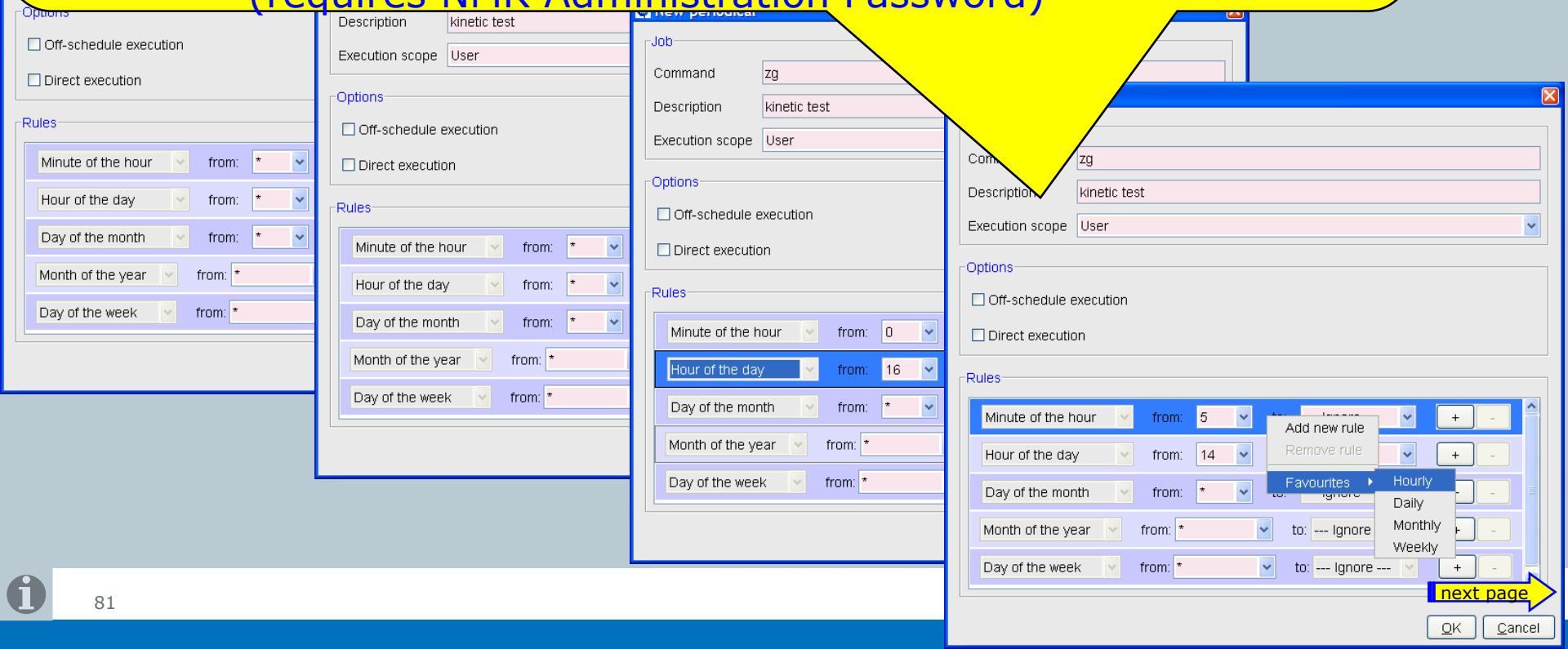


New command: **cron**

'Execution Scope'

user - defines a job for the current logged in user

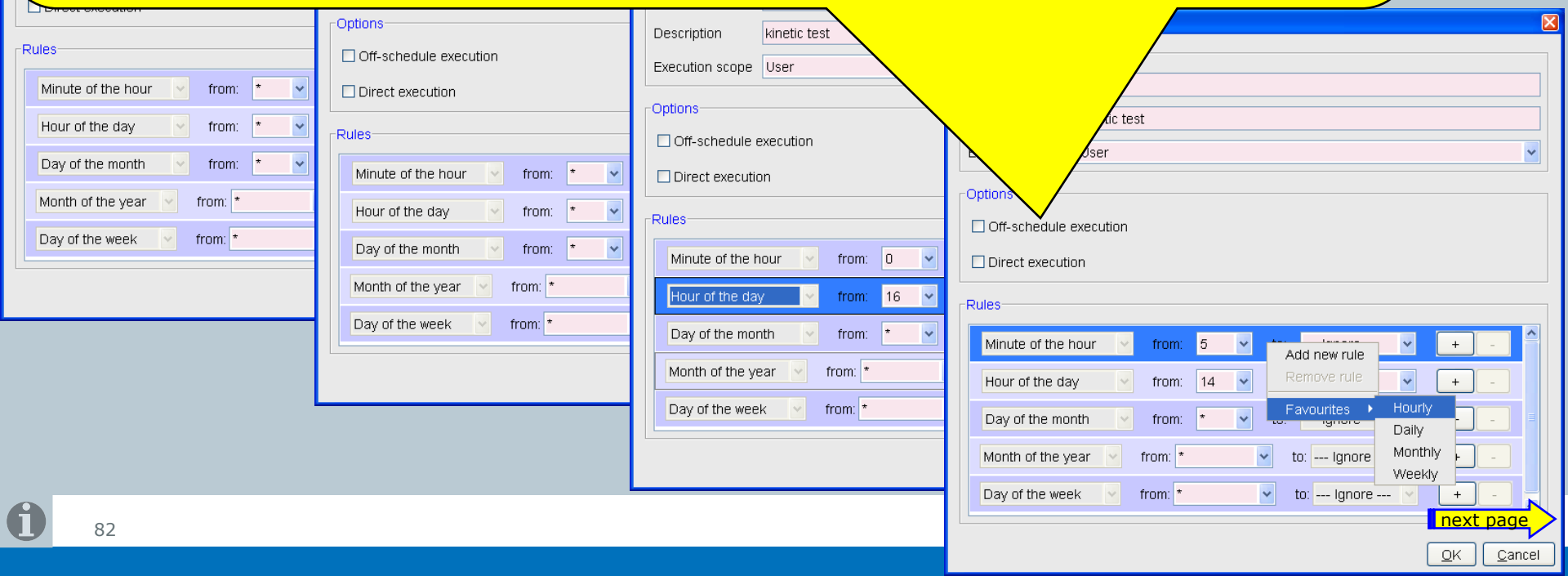
TopSpin - defines a job which should be executed independent of the current logged in user (requires NMR Administration Password)



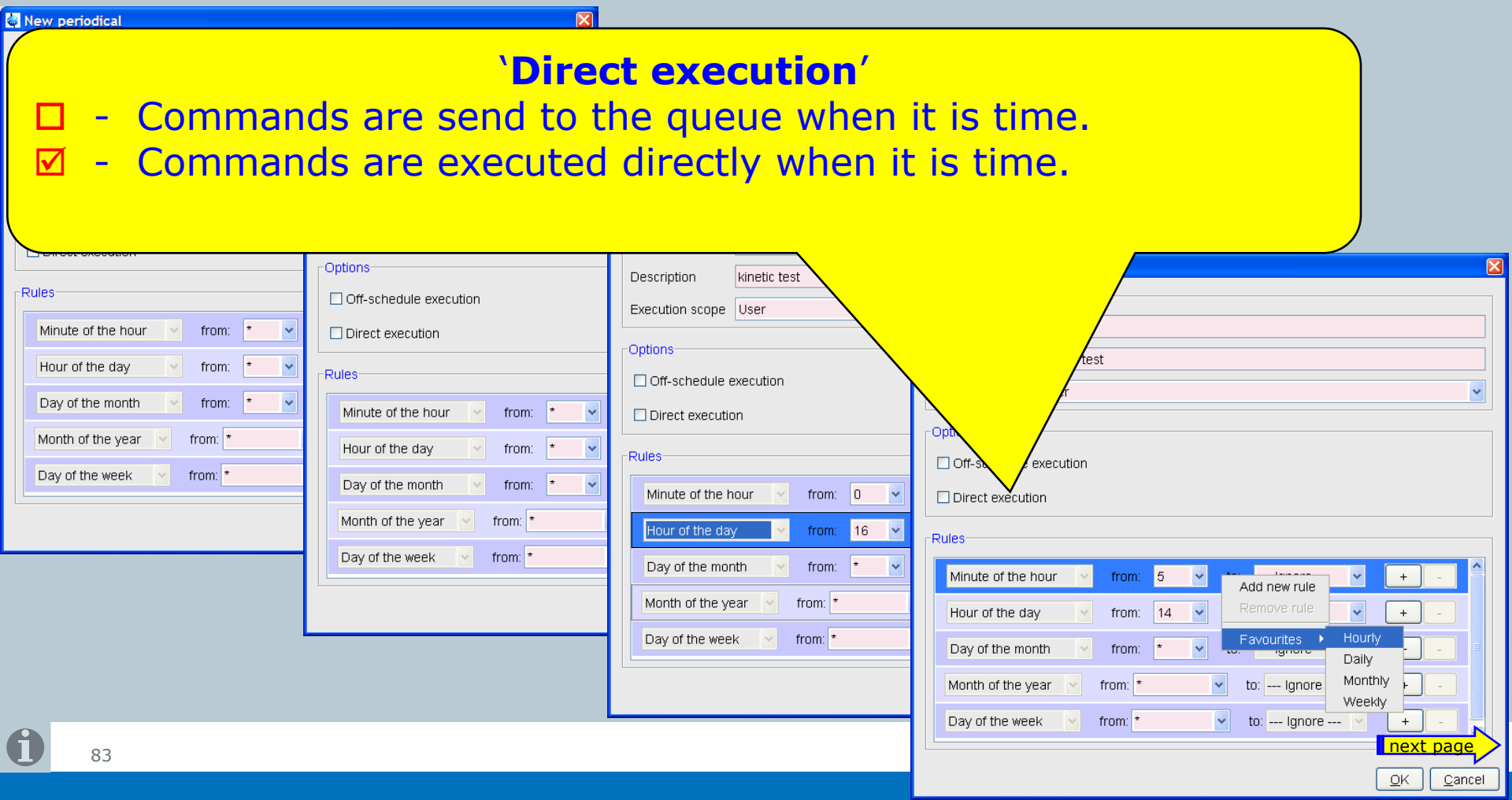
New command: **cron**

'Off-schedule execution'

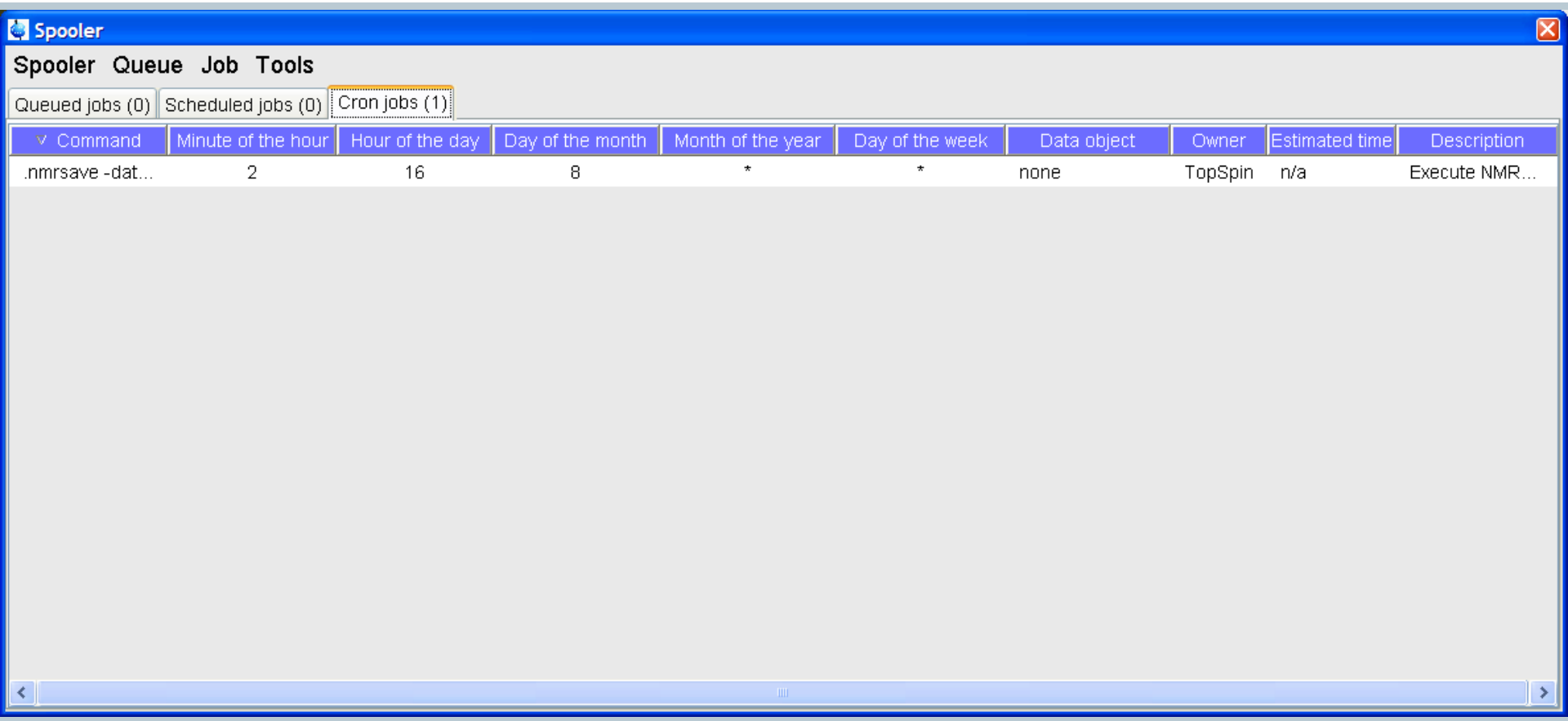
- ☐ - Jobs are executed only when TopSpin is up and running.
- ☑ - The last one of a series which could not be executed because TopSpin did not run, will be executed when TopSpin is started.



New command: **cron**

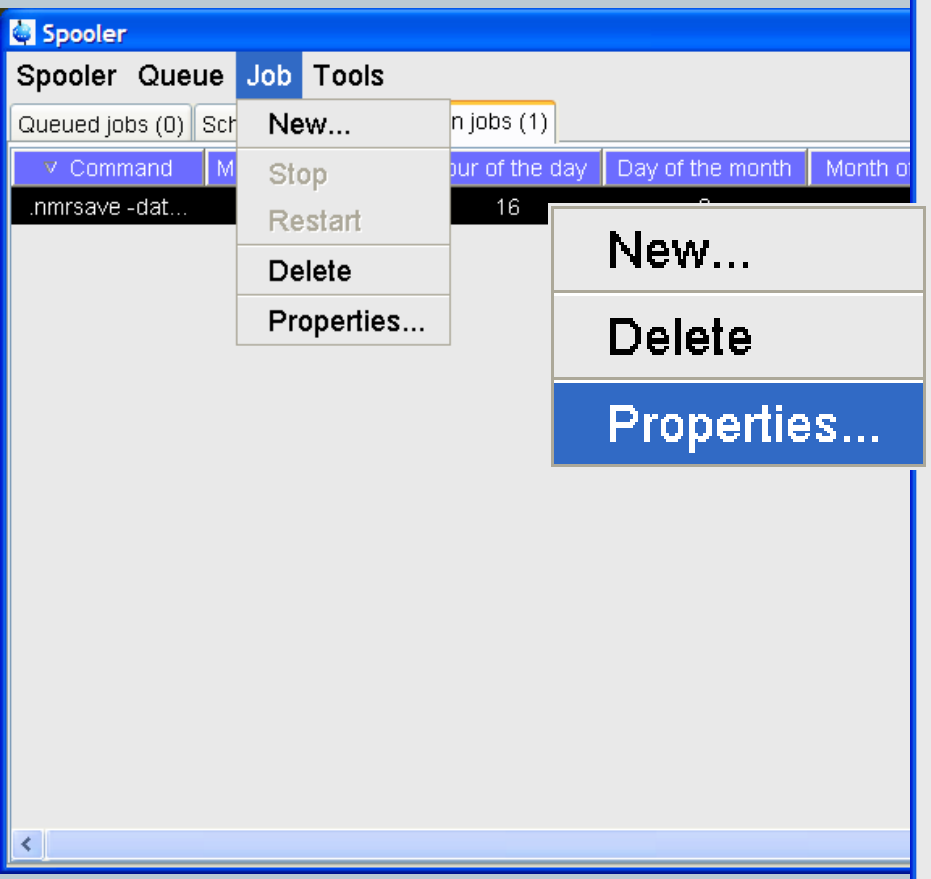


New commands: **edcron edqu edat**

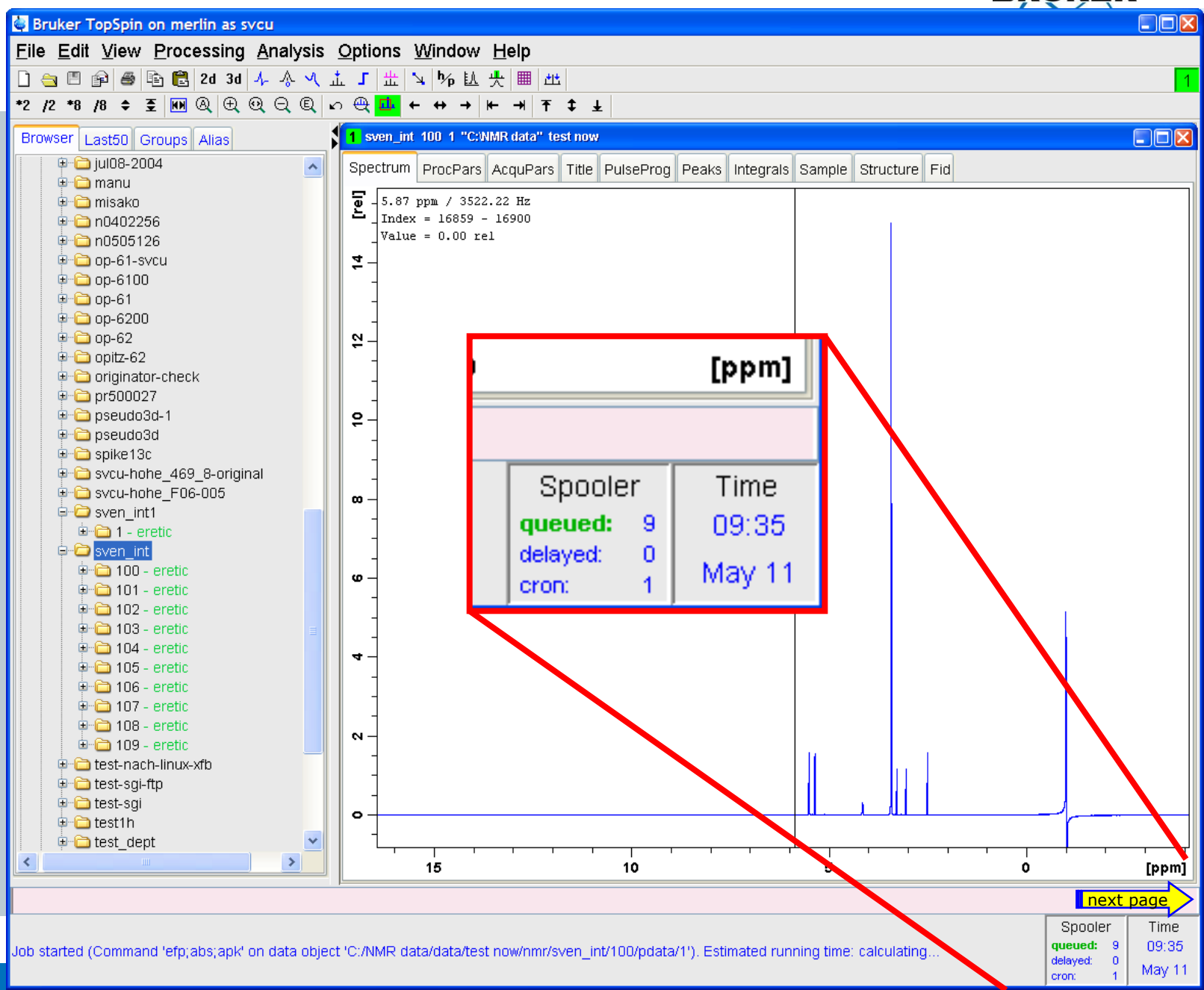


next page

New commands: **edcron**



Spooler in acquisition status bar



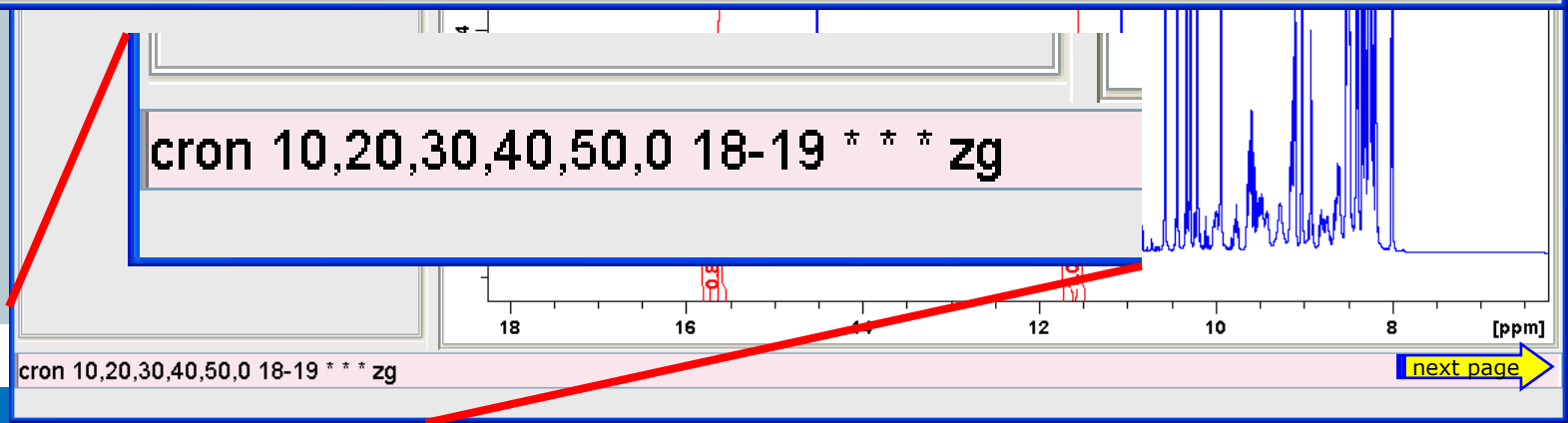
cron: command line options

Spooler

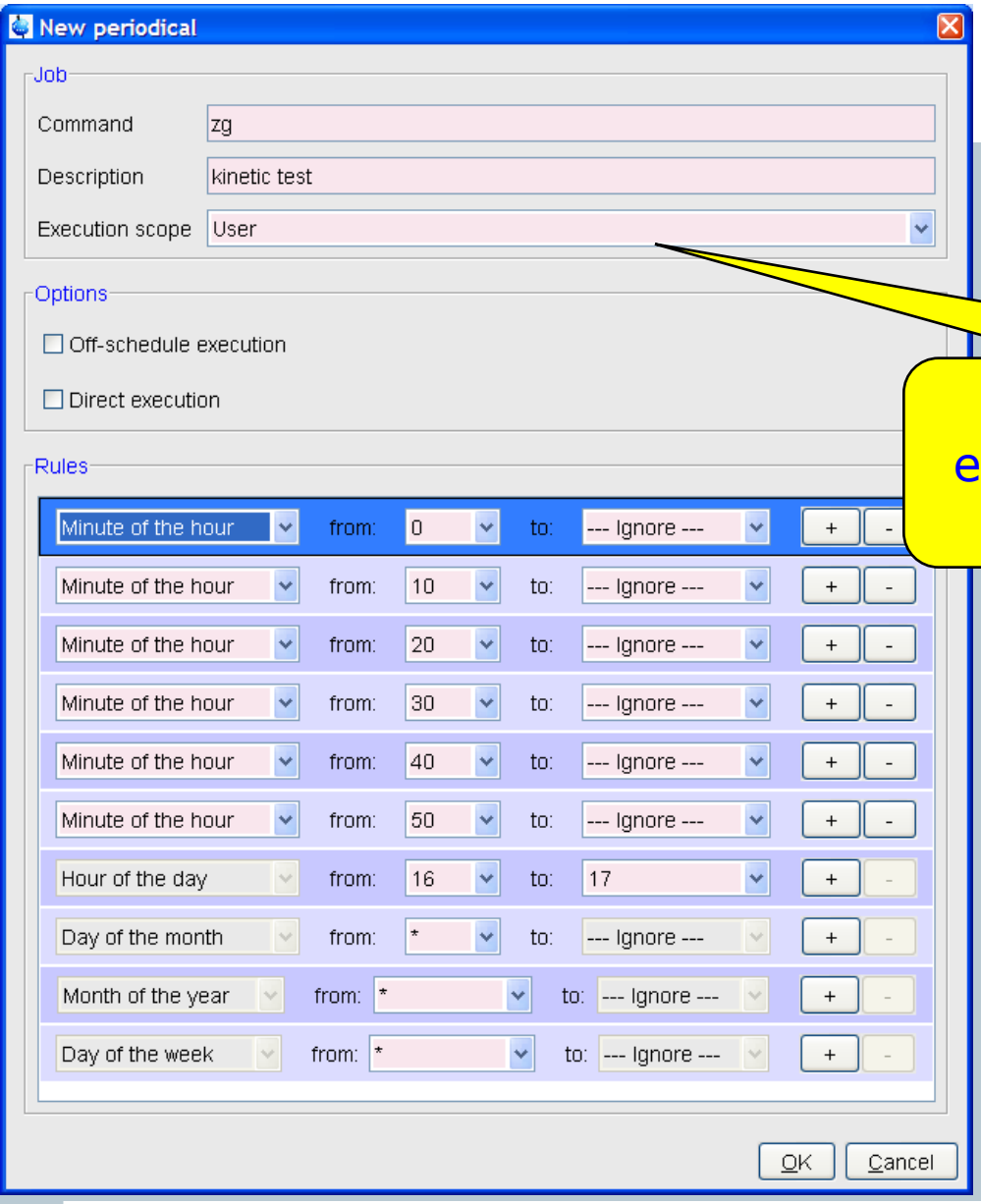
Spooler Job Tools

Queued jobs (0) | Scheduled jobs (0) | Cron jobs (2)

Command	Data object	Owner	Description	Minute of the hour	Hour of the day	Day of the month	Month of the year	Day of the week
zg	F:/Bruker/TopSpin/data/guest/...	svcu	kinetic test	0,10,20,30,40,50	16-17	*	*	*
zg	F:/Bruker/TopSpin/data/guest/...	svcu		10,20,30,40,50,0	18-19	*	*	*



cron usage – an example

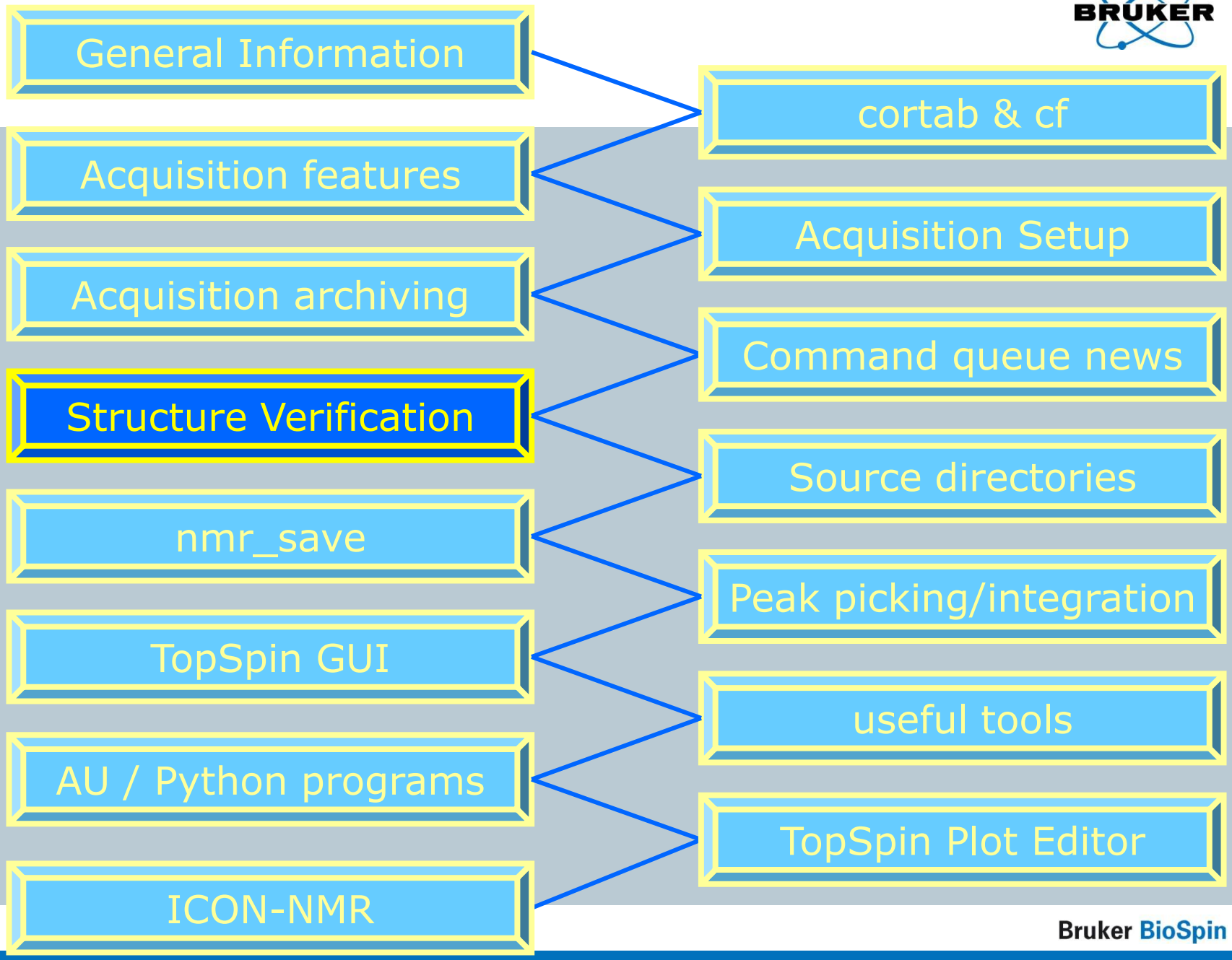


zg on current dataset will be executed every 10 minutes between 4 pm and 5 pm.

another example later on

next page

Content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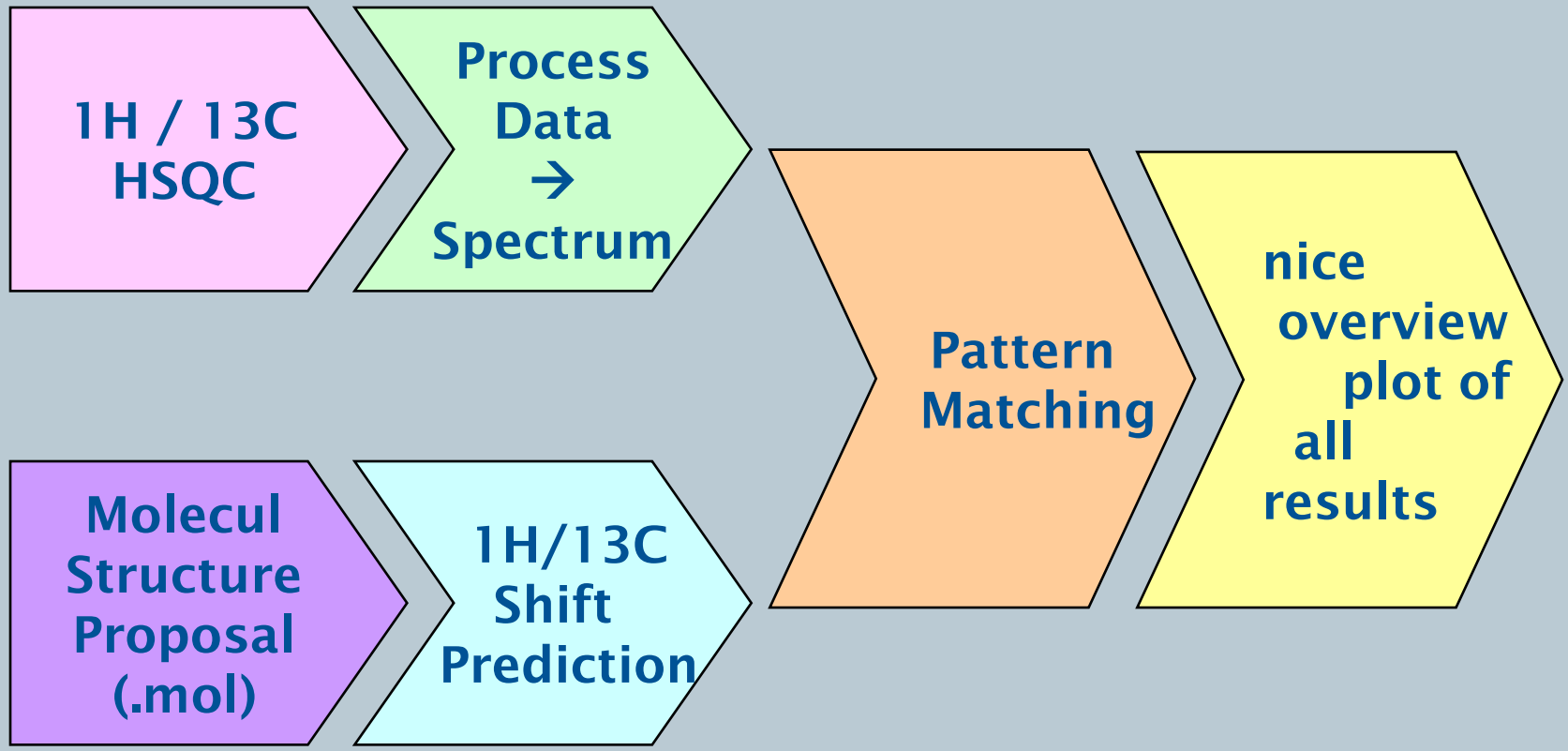
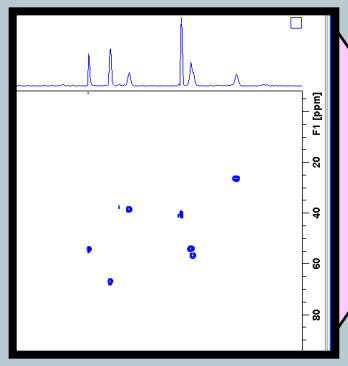
TopSpin Plot Editor

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor

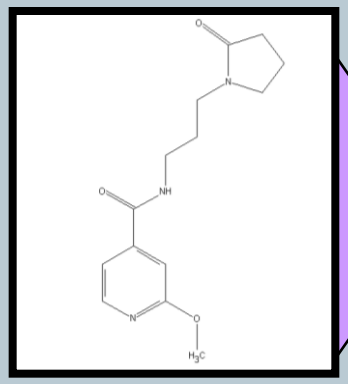


*Perch requires a separate license

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor

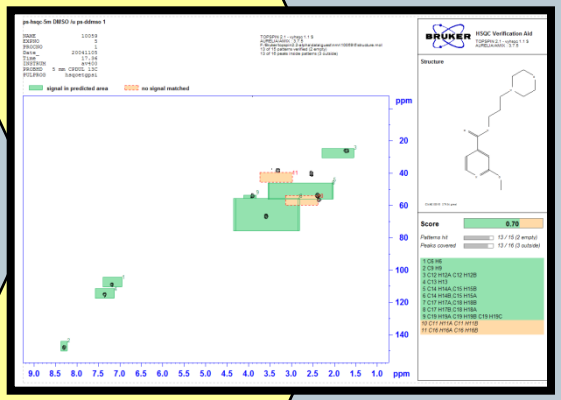


Process Data → Spectrum



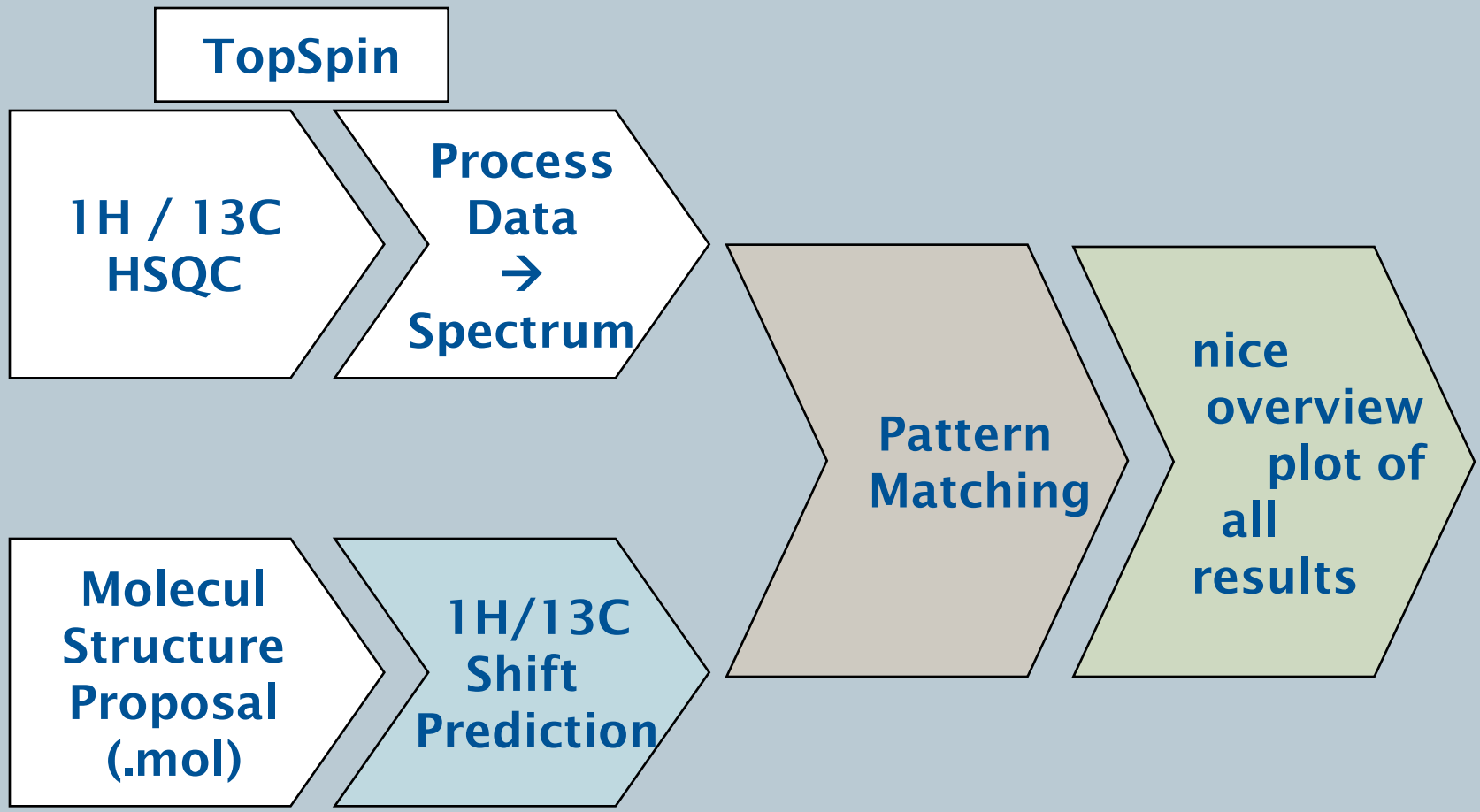
1H/13C Shift Prediction

Pattern Matching



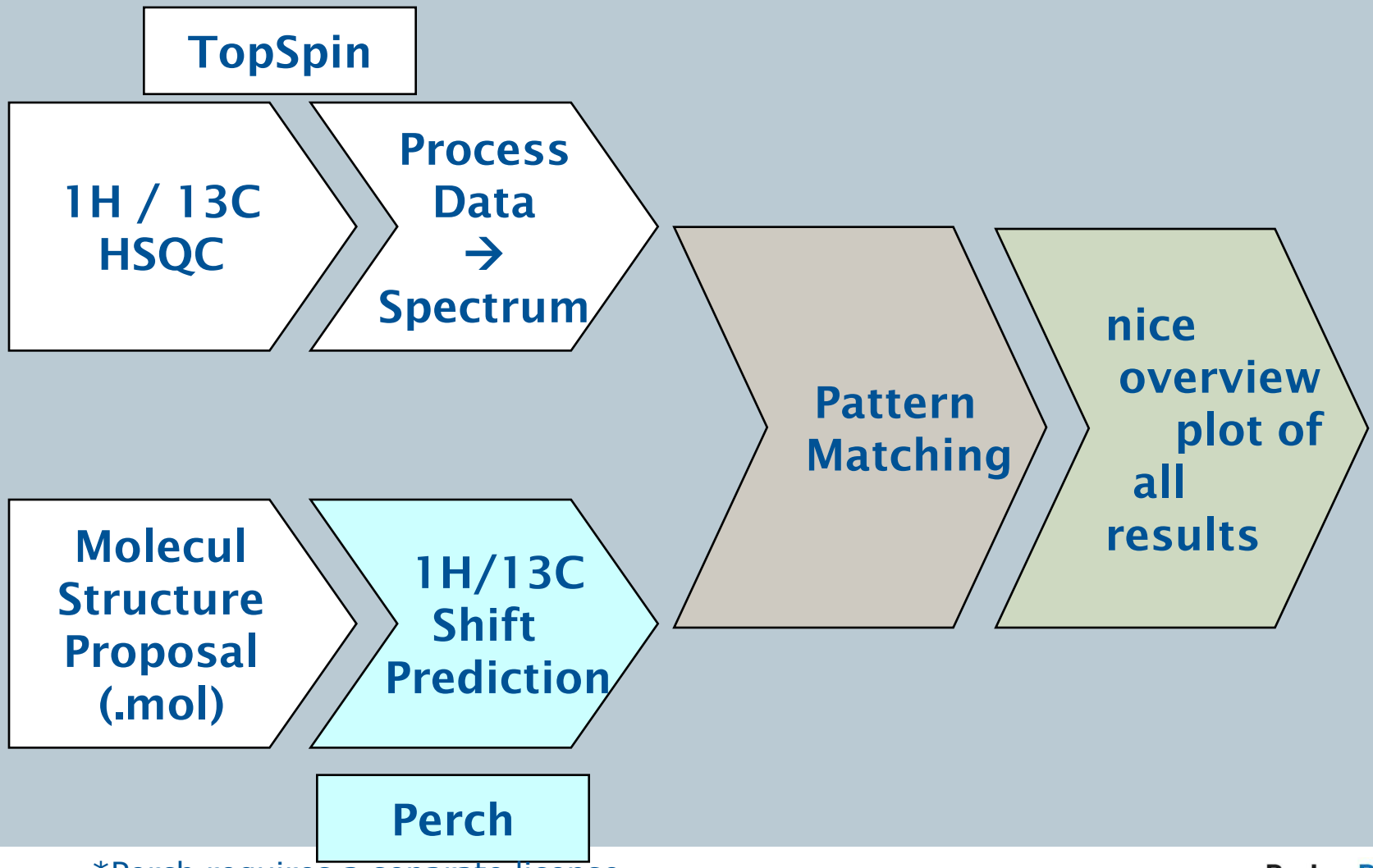
*Perch requires a separate license

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor



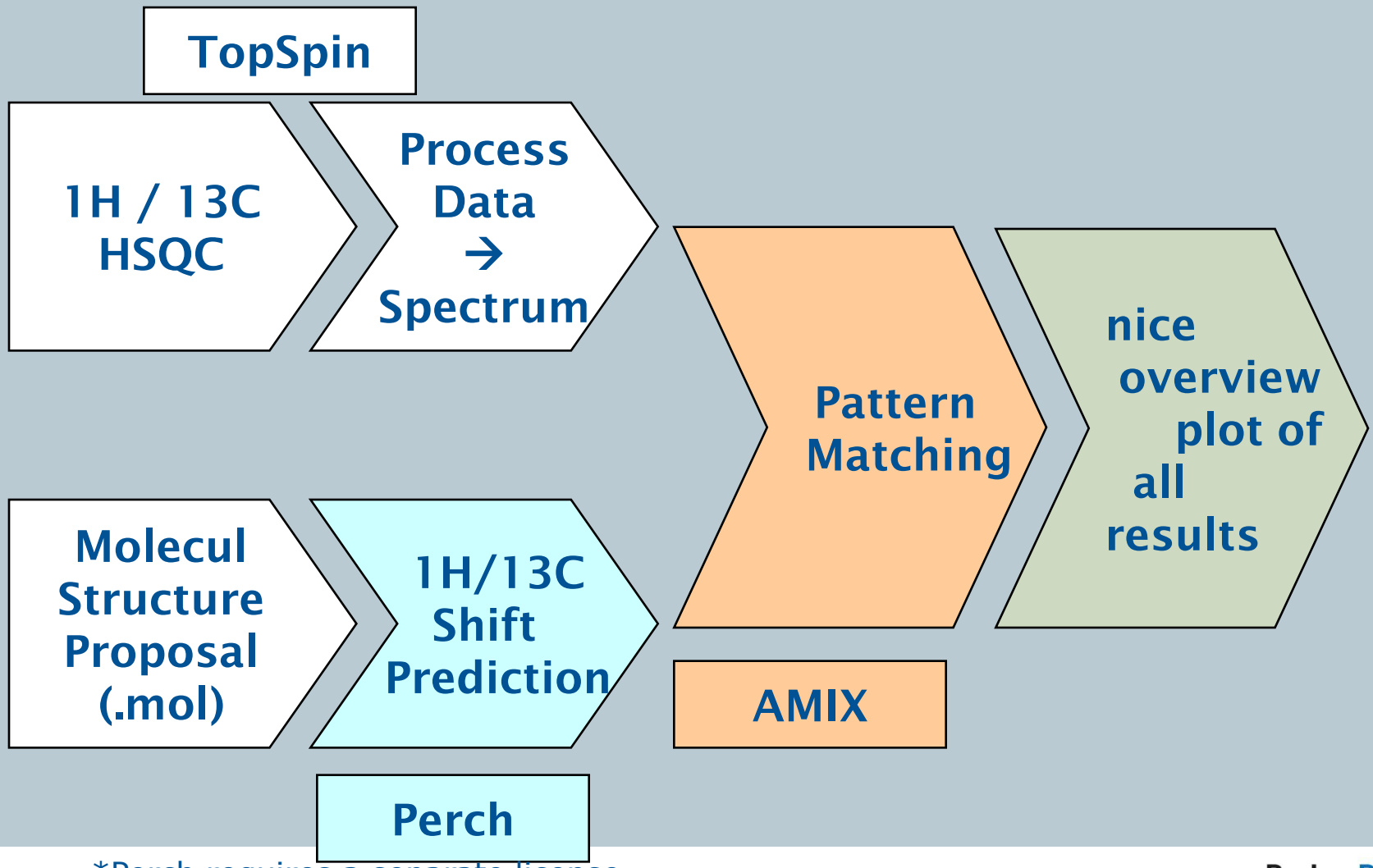
*Perch requires a separate license

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor



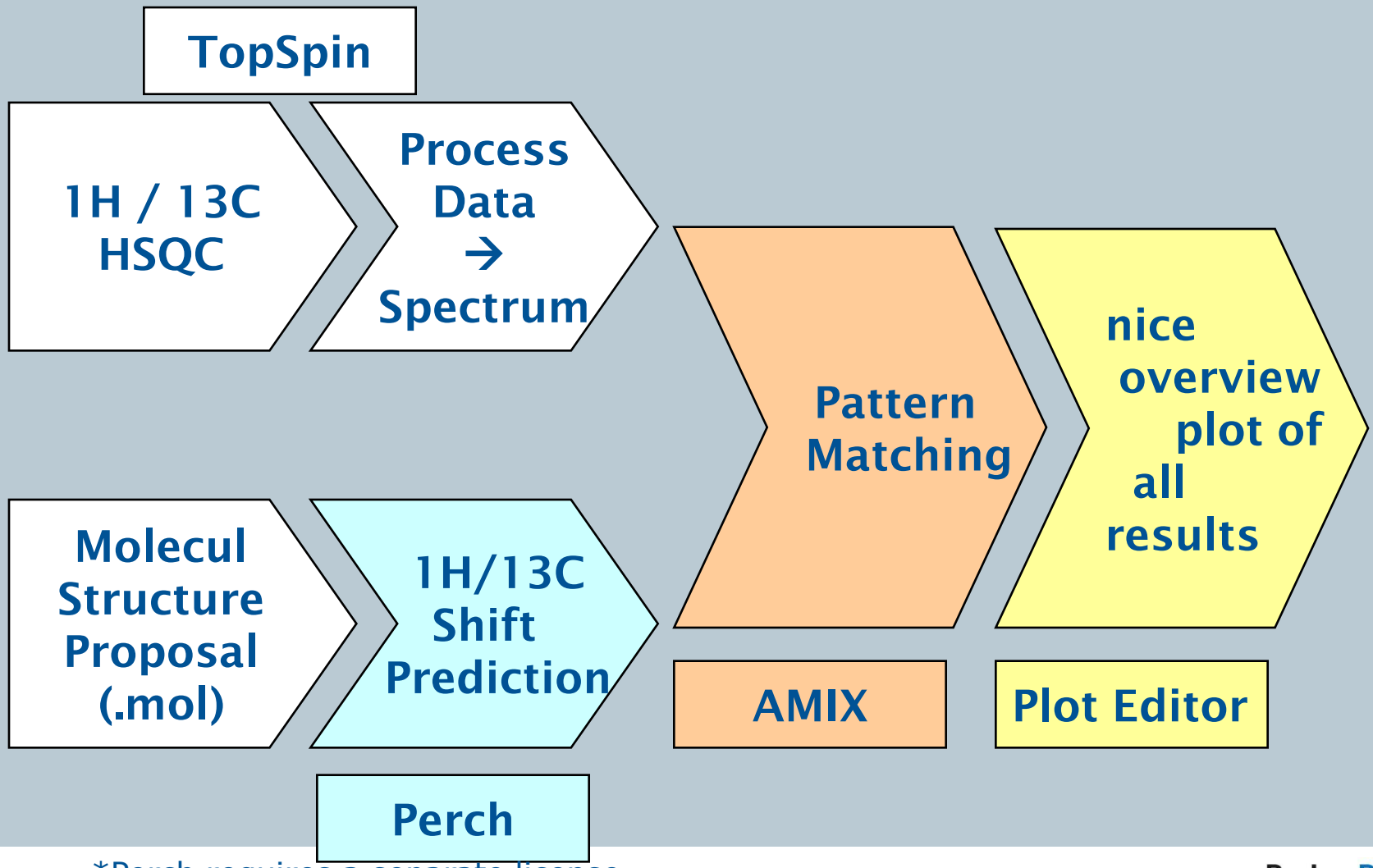
*Perch requires a separate license

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor



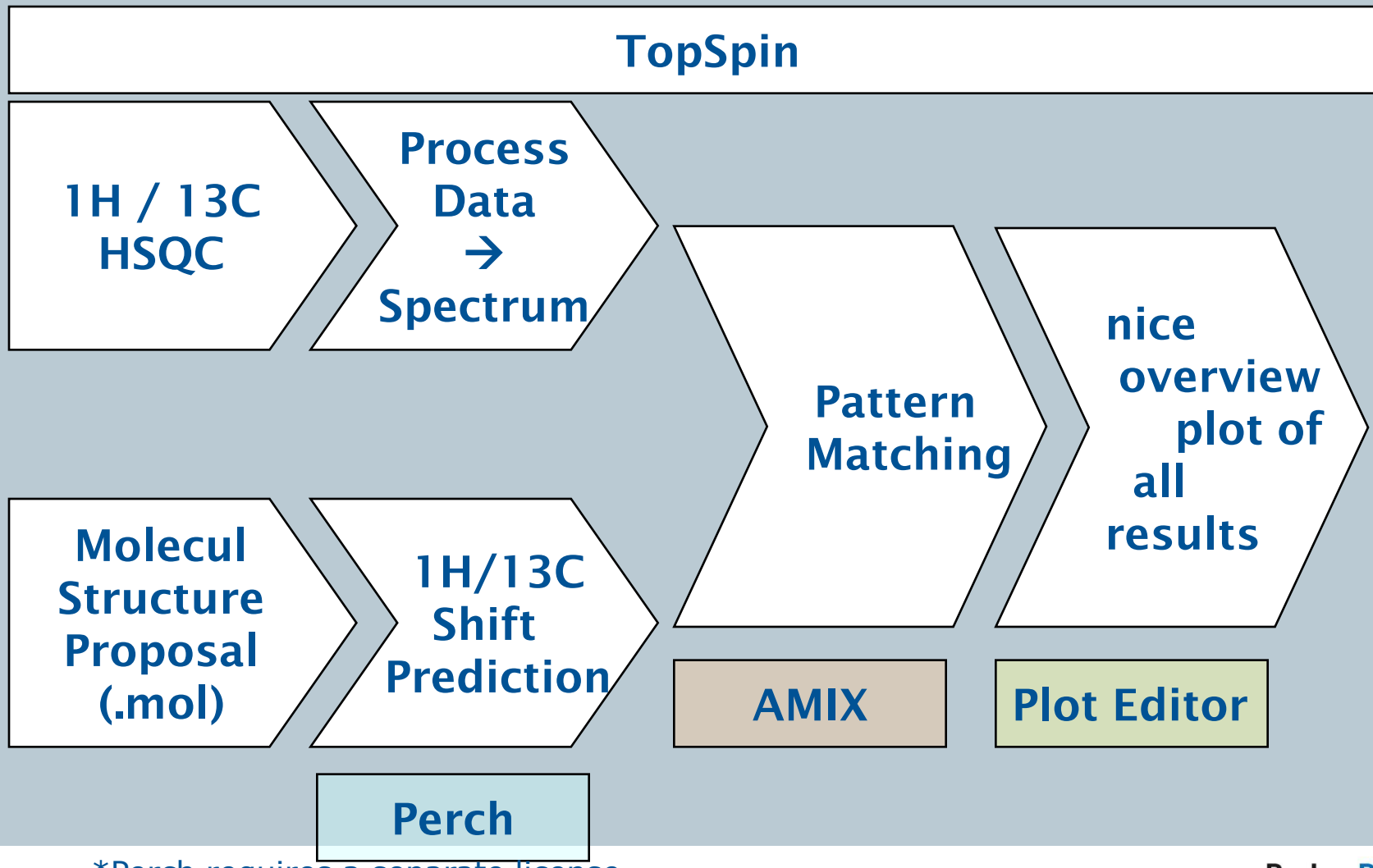
*Perch requires a separate license

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor



*Perch requires a separate license

Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor



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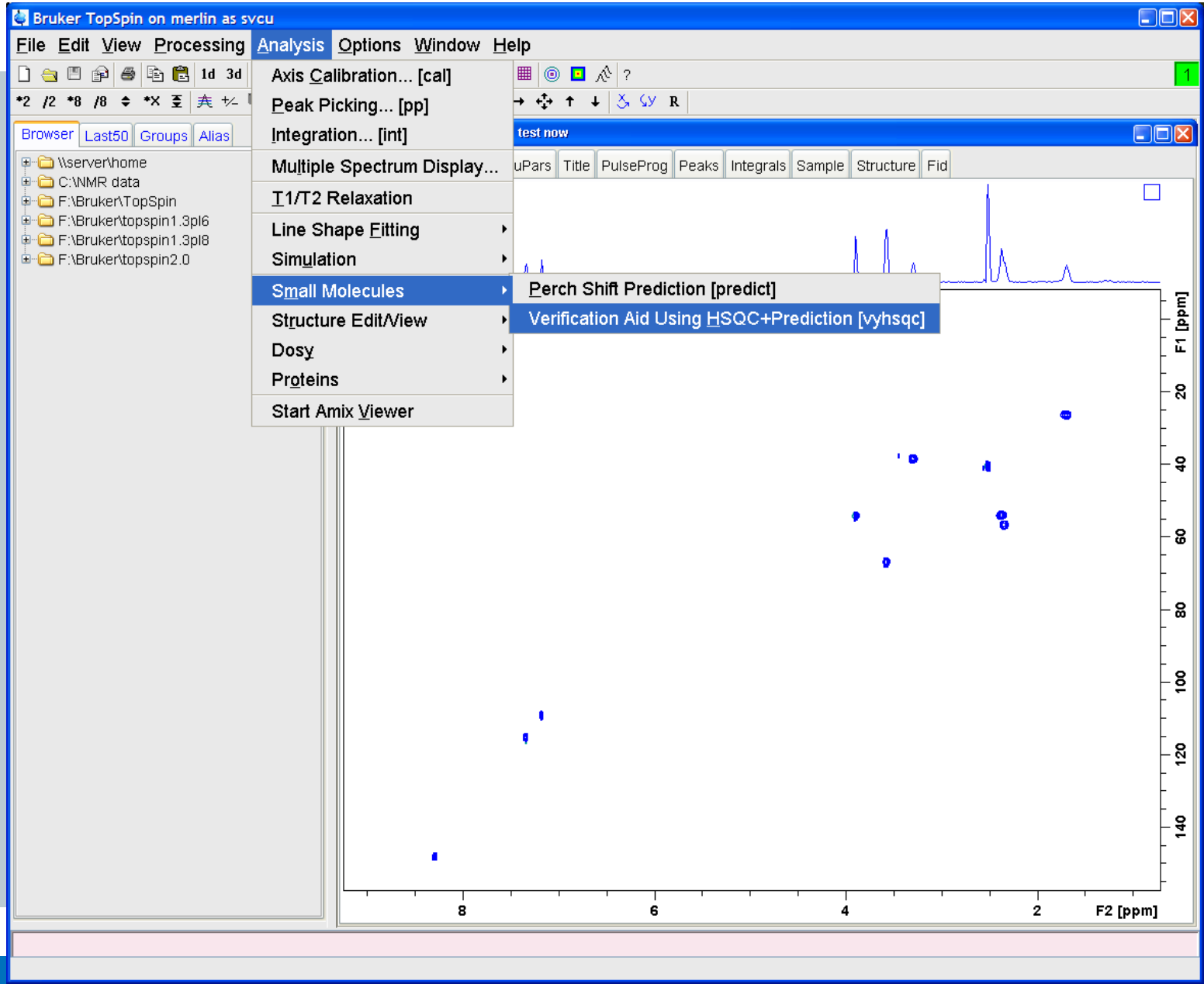
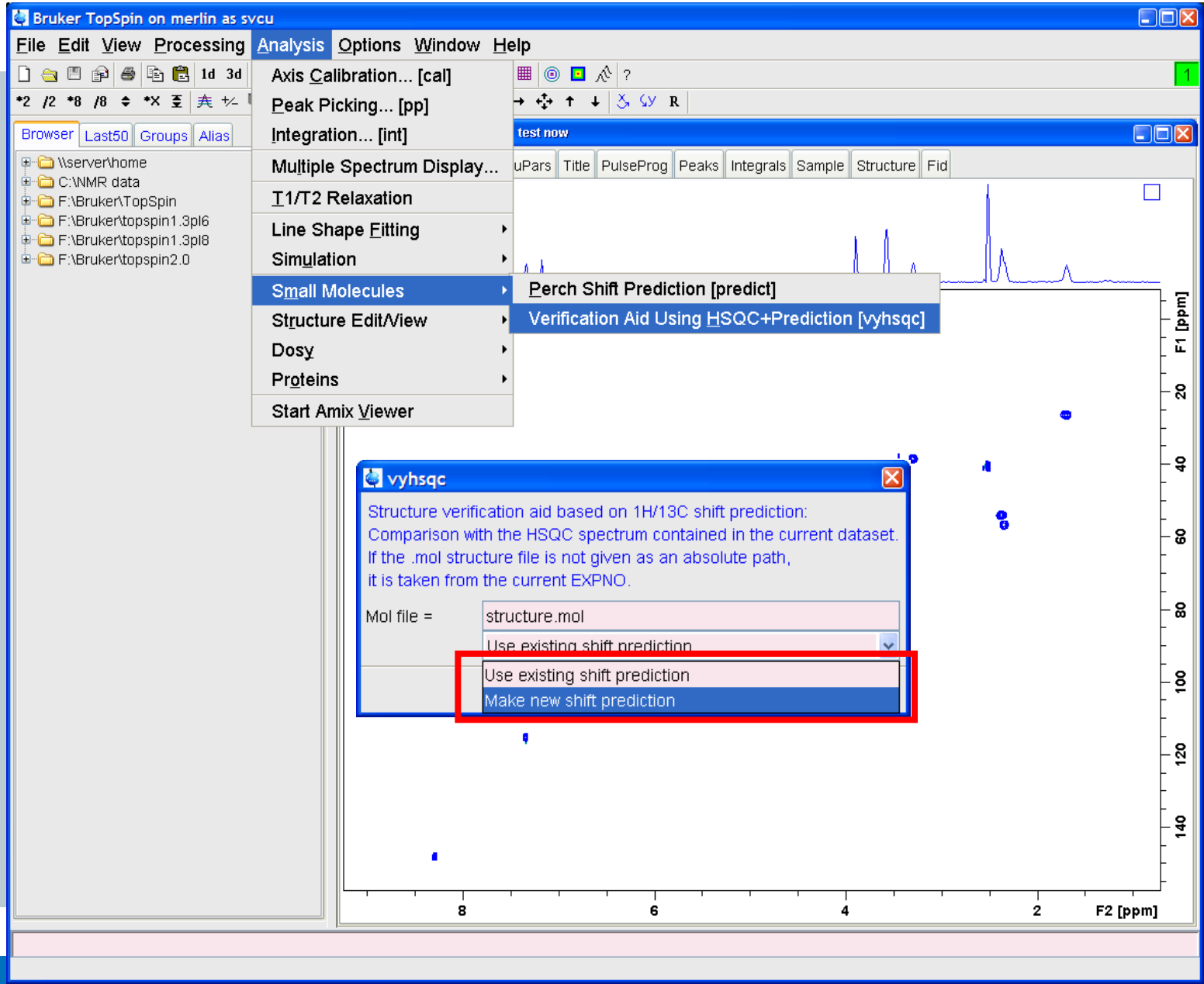
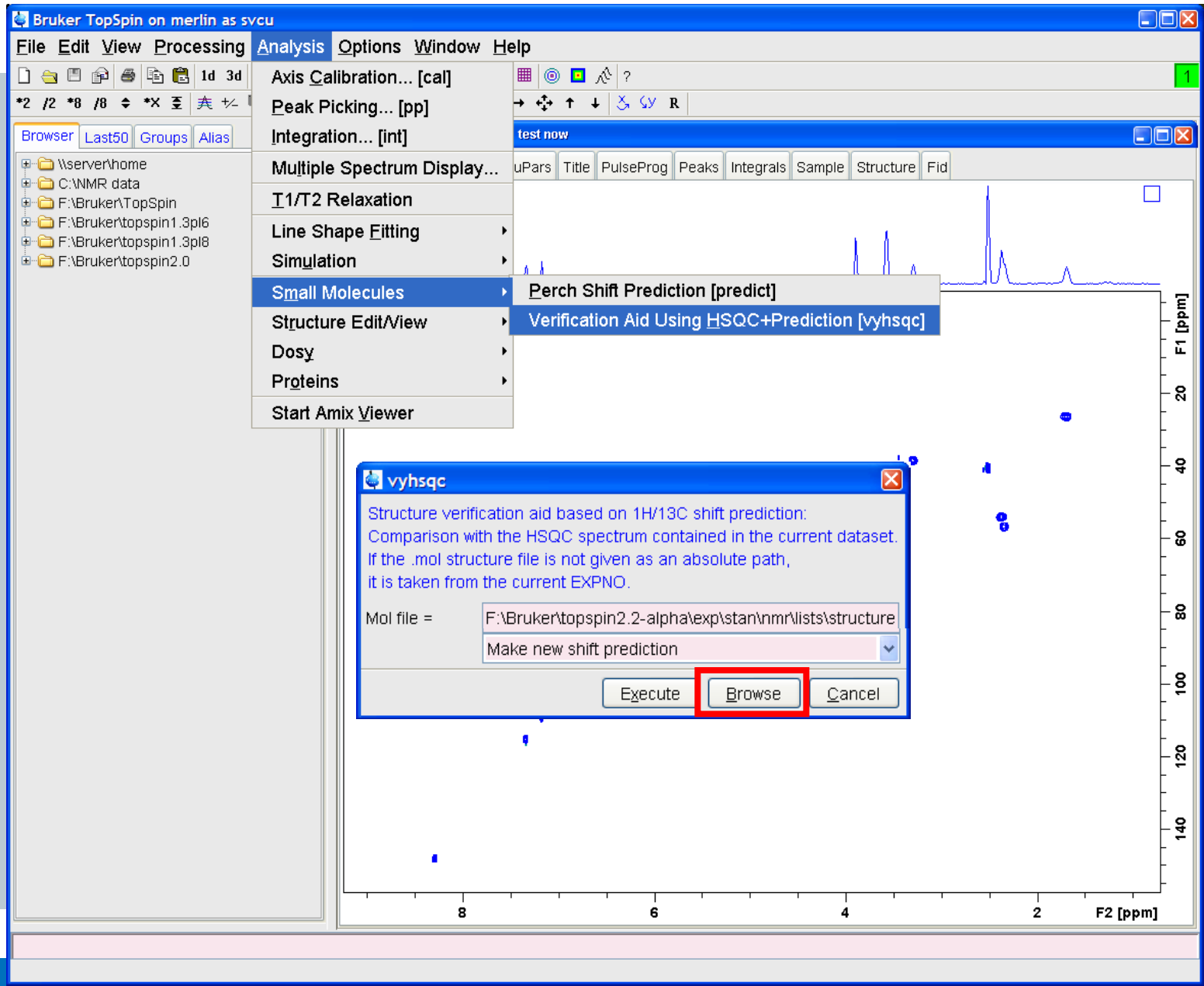
Structure Verification Aid



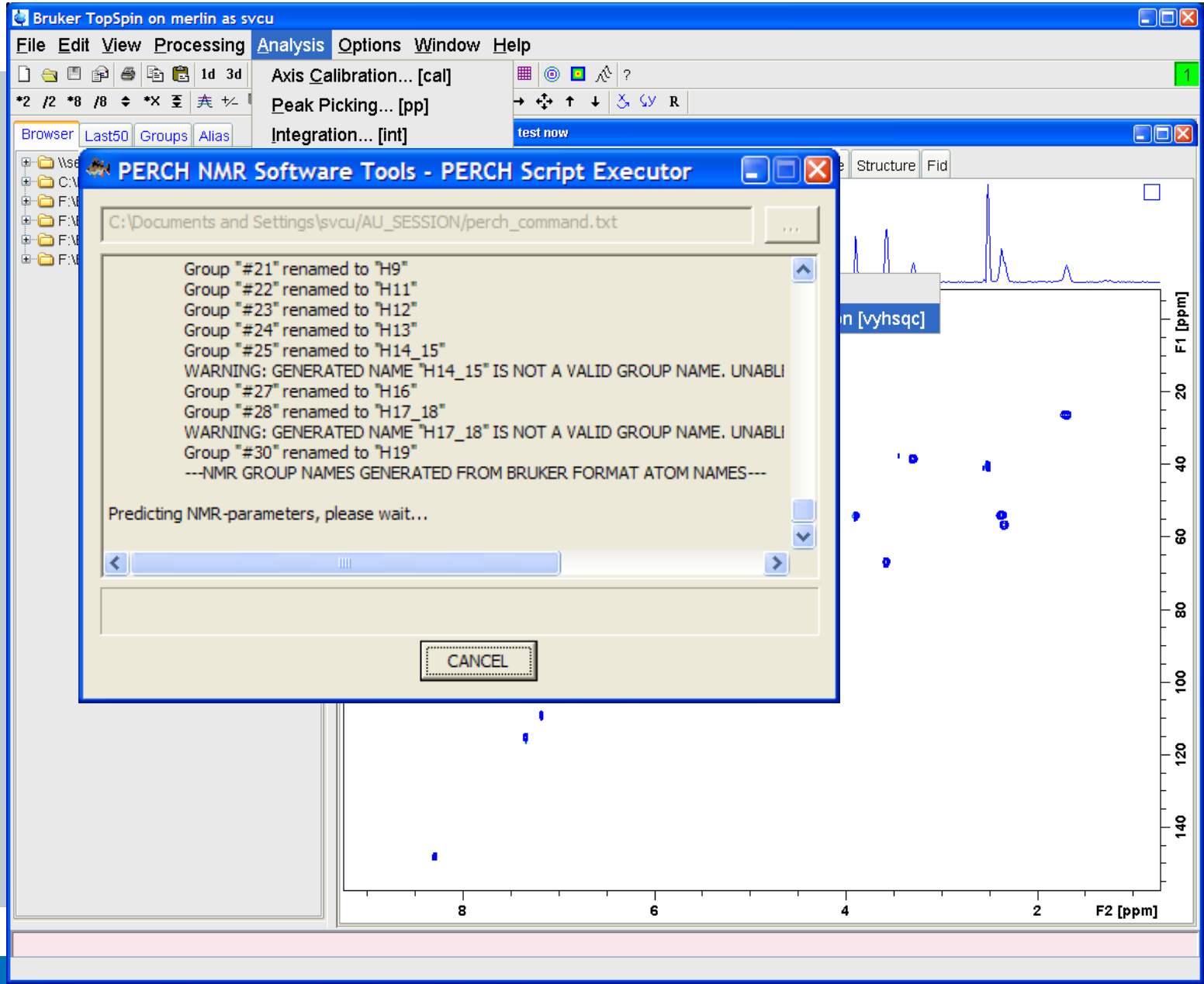
Structure Verification Aid



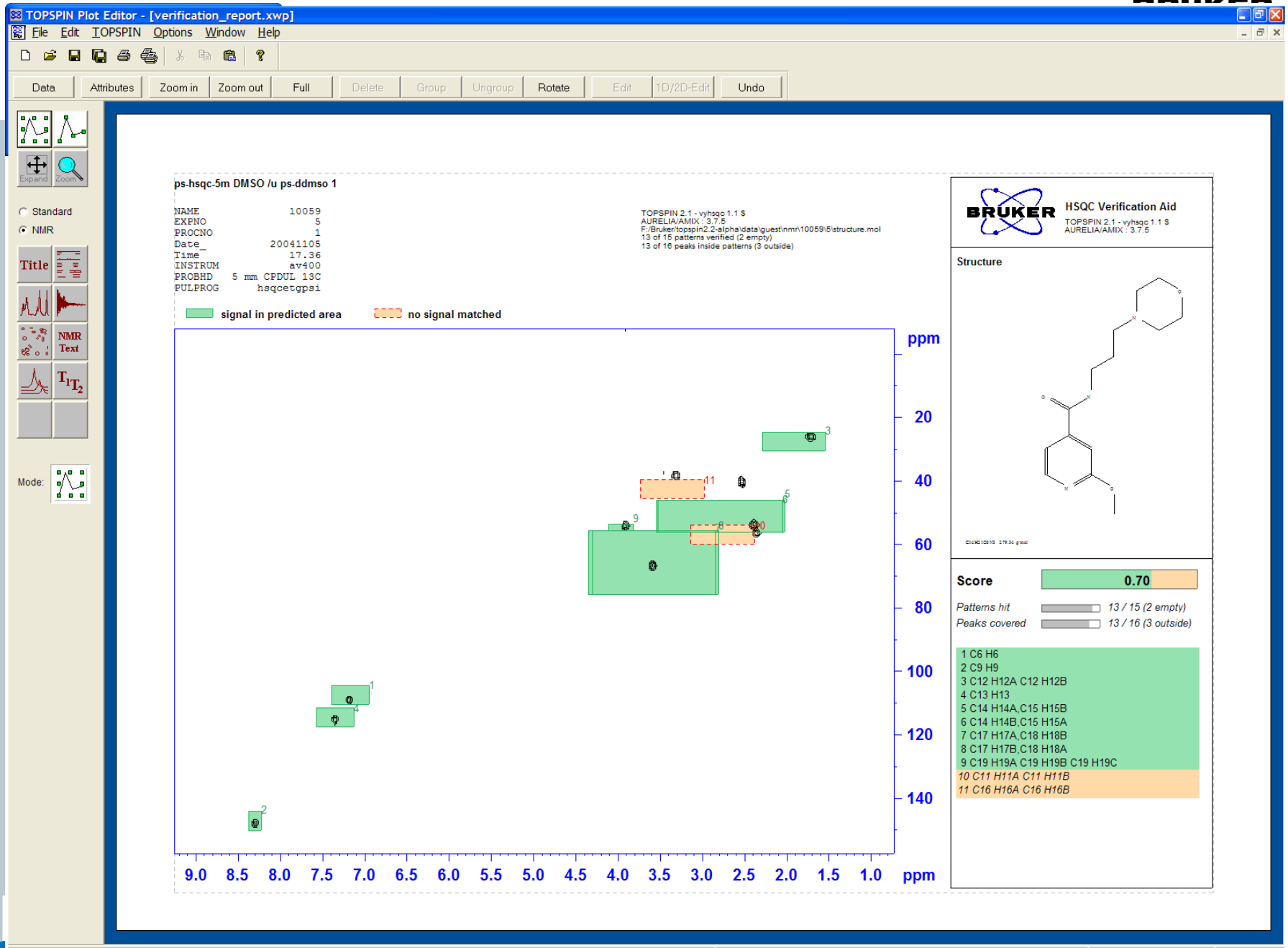
Structure Verification Aid



Structure Verification Aid



Structure Verification Aid



print out

and as PDF

C:\NMR data\data\test now\nmr\10059\5\pdata\1

File Edit View Favorites Tools Help

Back Search Folders

Address C:\NMR data\data\test now\nmr\10059\5\pdata\1 Go

Folders

- nmr
  - ~TEMP
  - 13C_Spektrum
  - 13c-dept
  - 30ml
  - 30ml-2
  - 50ml
  - 50ml-2
  - 62
  - 62orig
  - 70ml
  - 10059
    - 5
      - pdata
        - 1
        - 1000
        - 1001
        - 1002
  - 10060
  - 10061
  - 2006000099067
  - 2006000099068
  - cunskis-demo
  - DRU dataset
  - elin
  - elin3.fid
  - franz
  - friedrich
  - heinecke

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2ir	4.096 KB
2ri	4.096 KB
2rr	4.096 KB
10059.MMS	8 KB
Amix.prot	1 KB
Arr.fb	4 KB
auditp.txt	2 KB
clevels	2 KB
curdat2	1 KB
email_10059_5_1.pdf	40 KB
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loc_level	1 KB
portf	1 KB
proc	2 KB
proc2	2 KB
proc2s	2 KB
procs	2 KB
structure.emf	4 KB
structure.mol	2 KB
title	1 KB
verification_log.txt	3 KB
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verification_report_10059.pdf	93 KB
verification_summary.txt	1 KB
verify.amix	1 KB
verify_10059.pred	6 KB
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verify_result.txt	4 KB
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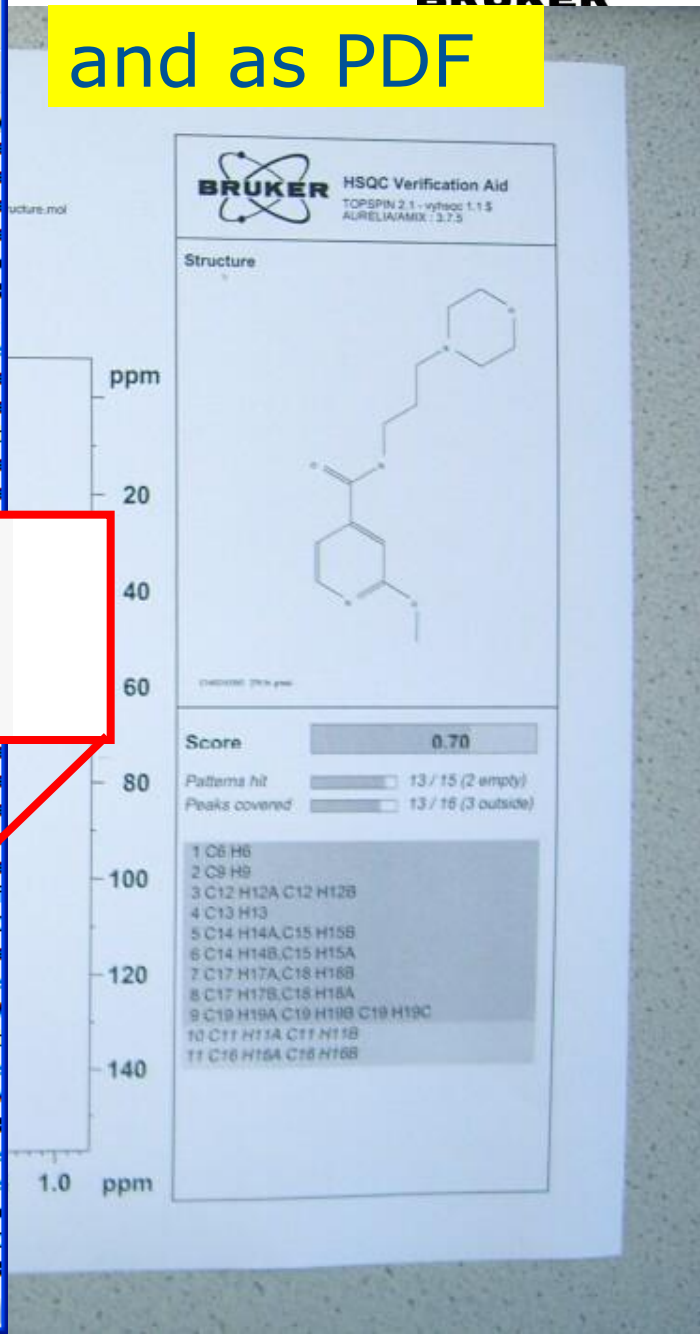
verification_report.xwp

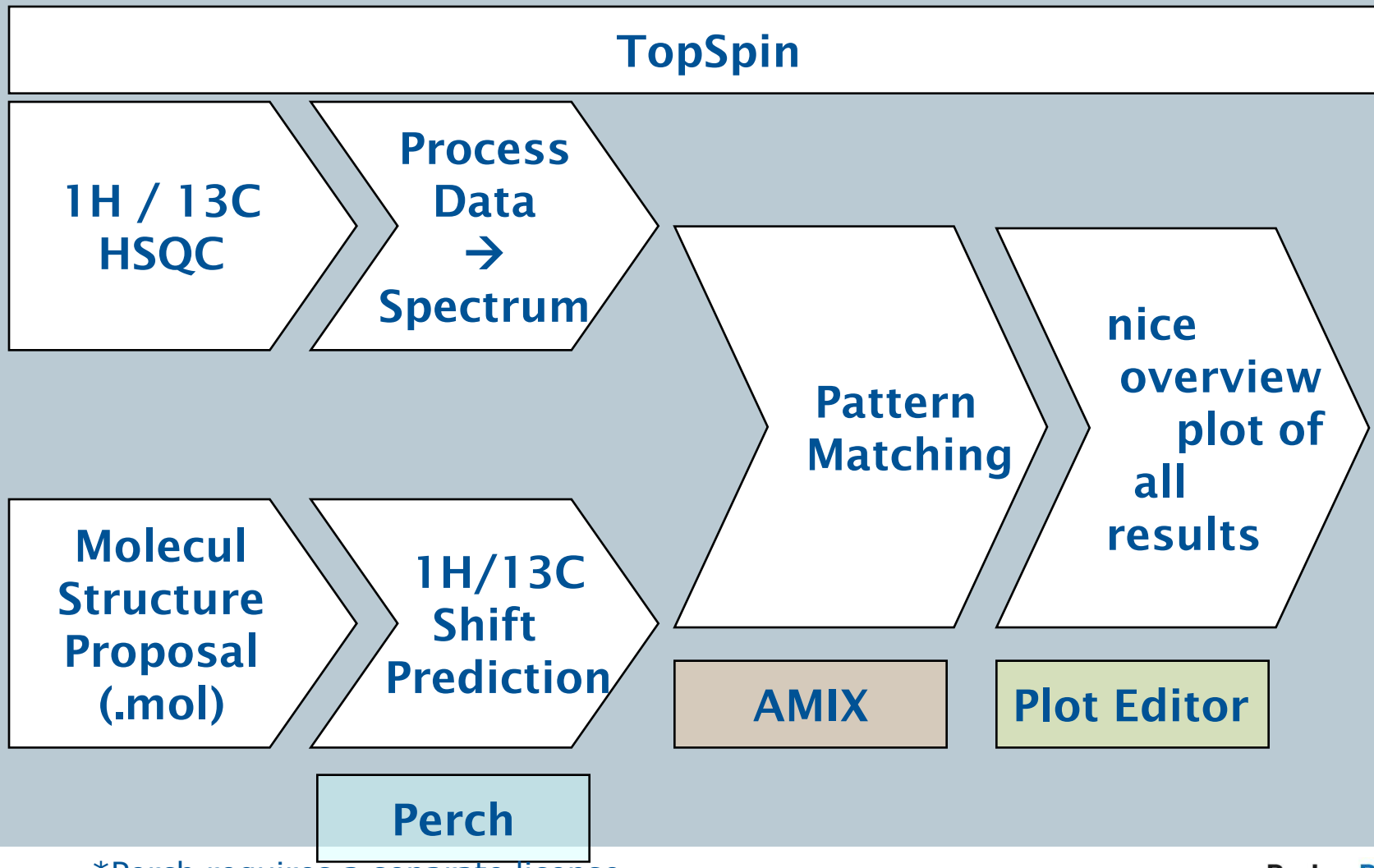
verification_report_10059.pdf

verification_summary.txt



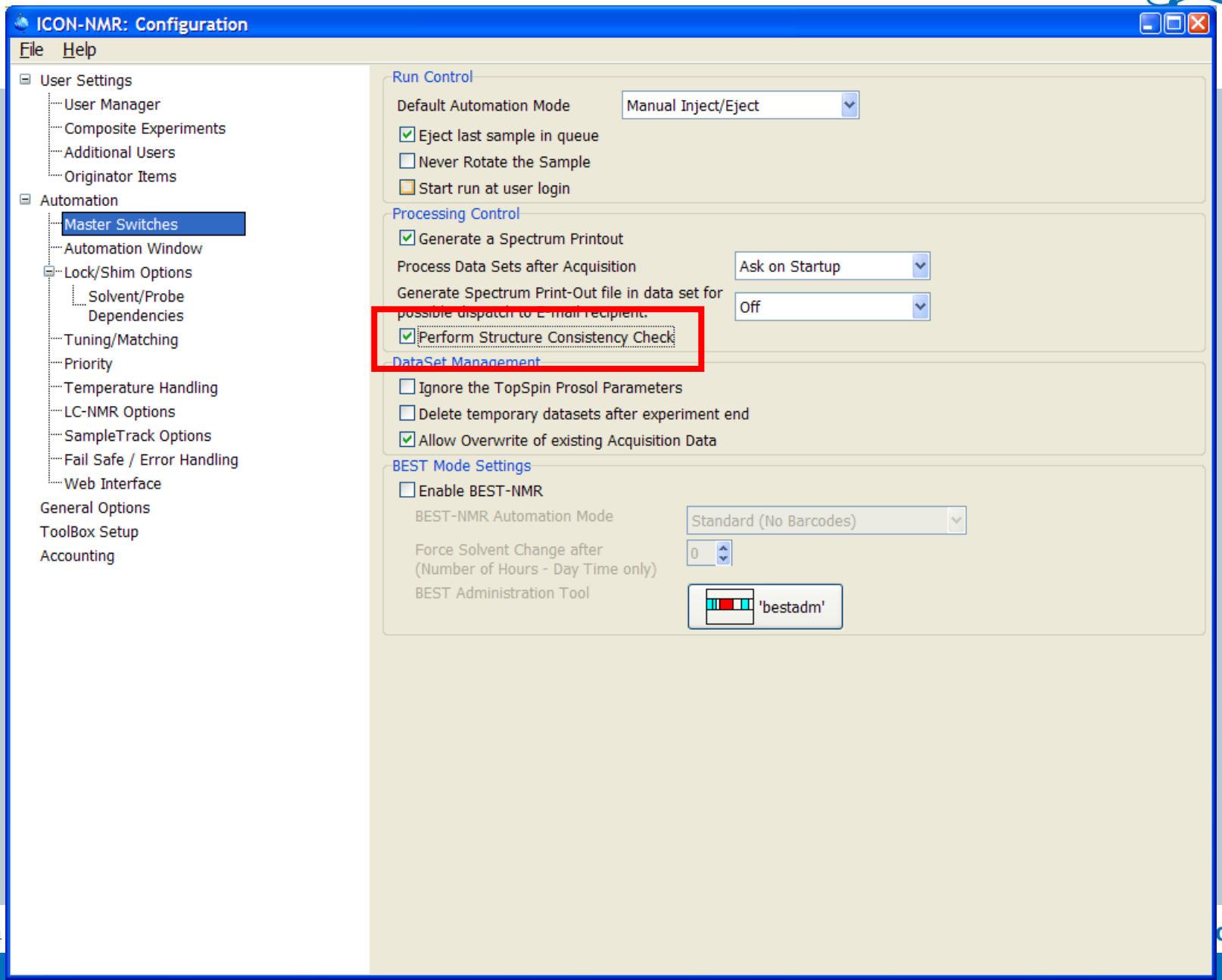
Teamwork:
TopSpin/Perch*/AMIX/TS Plot Editor

ICON-NMR

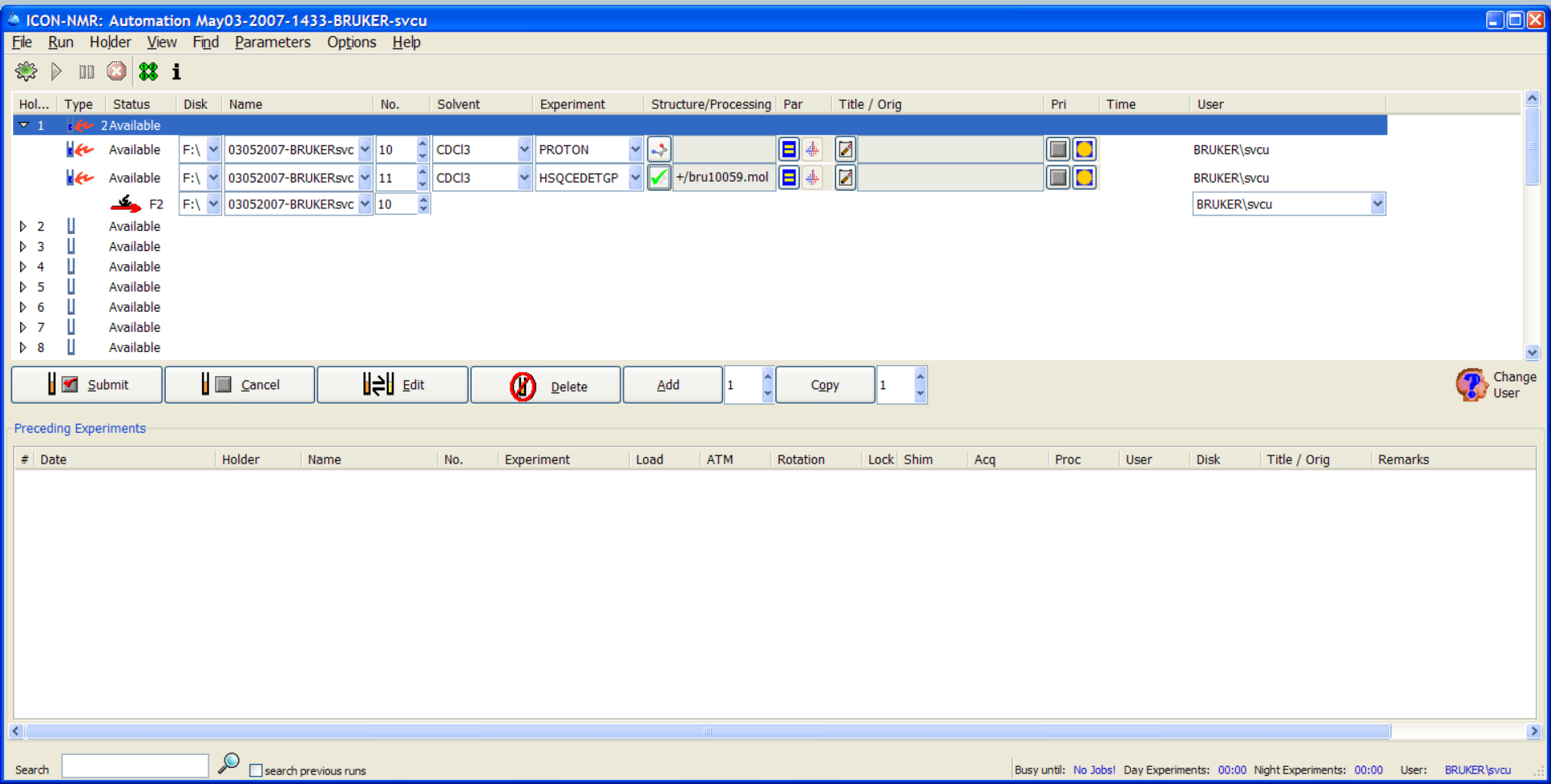


*Perch requires a separate license

Structure Verification Aid



Structure Verification Aid



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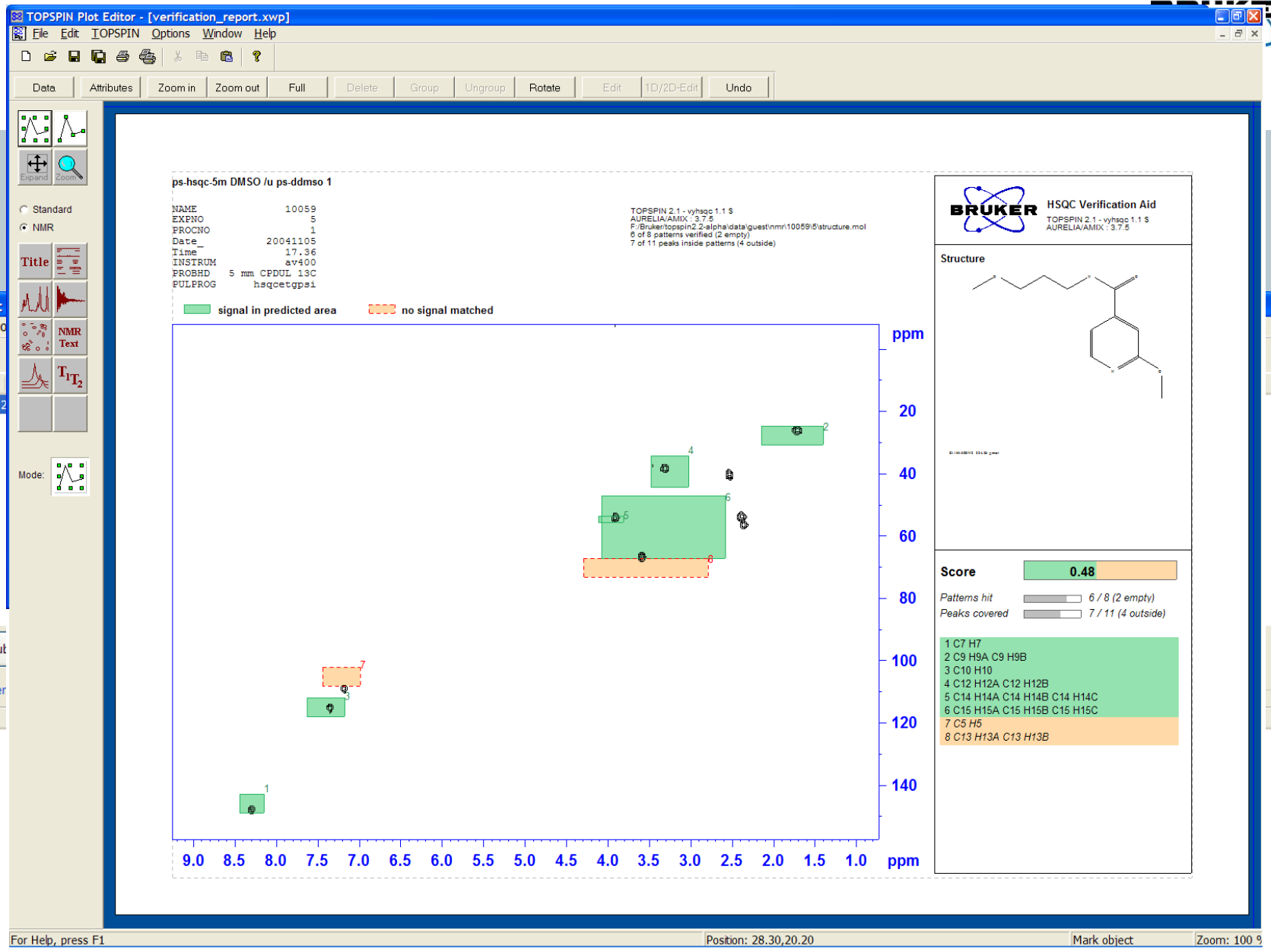
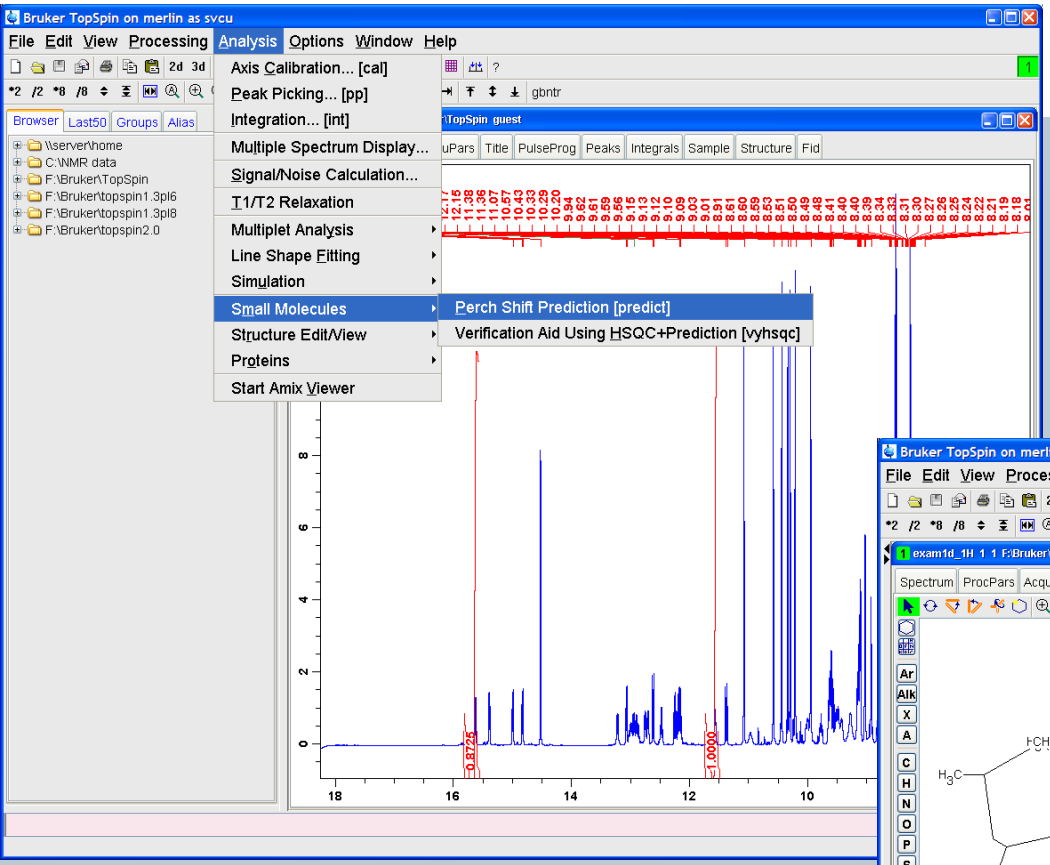
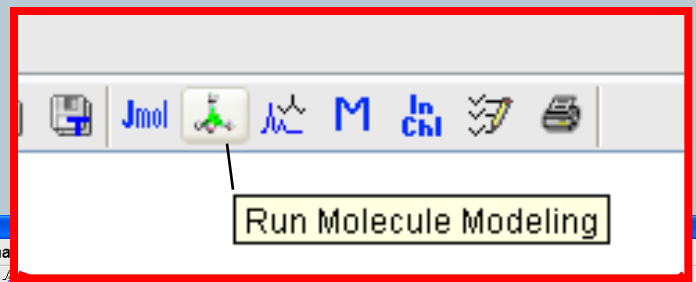
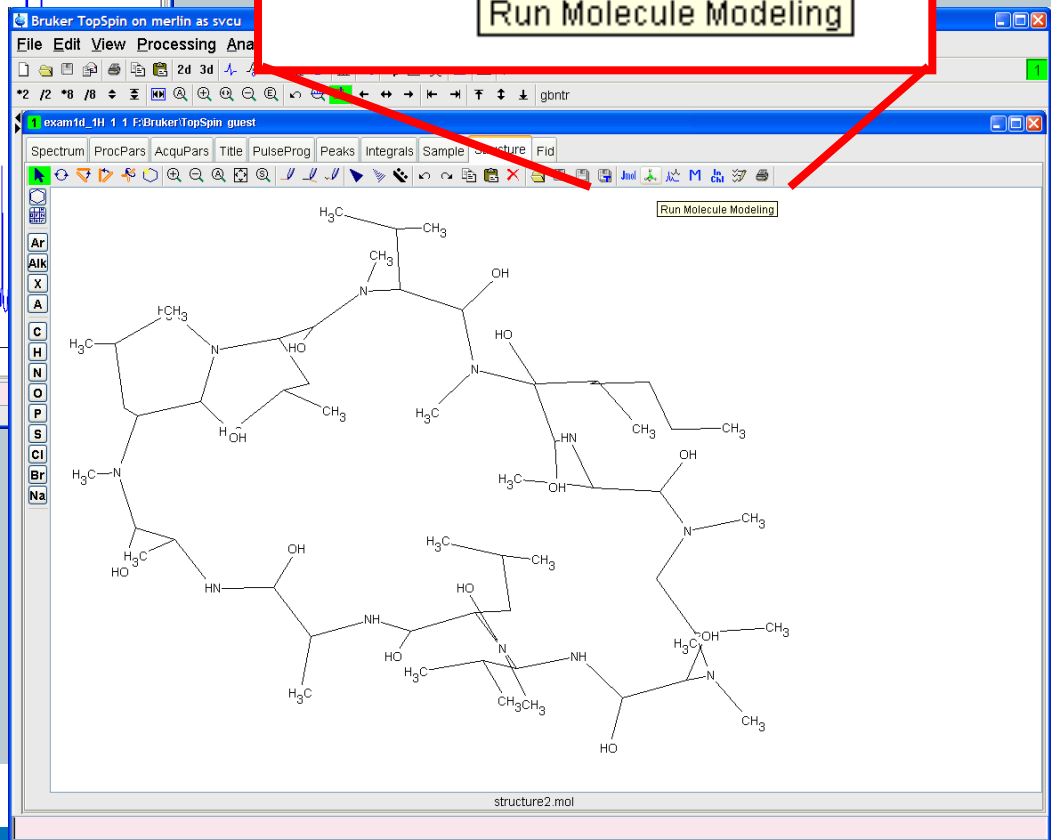


Other Perch* features within TopSpin

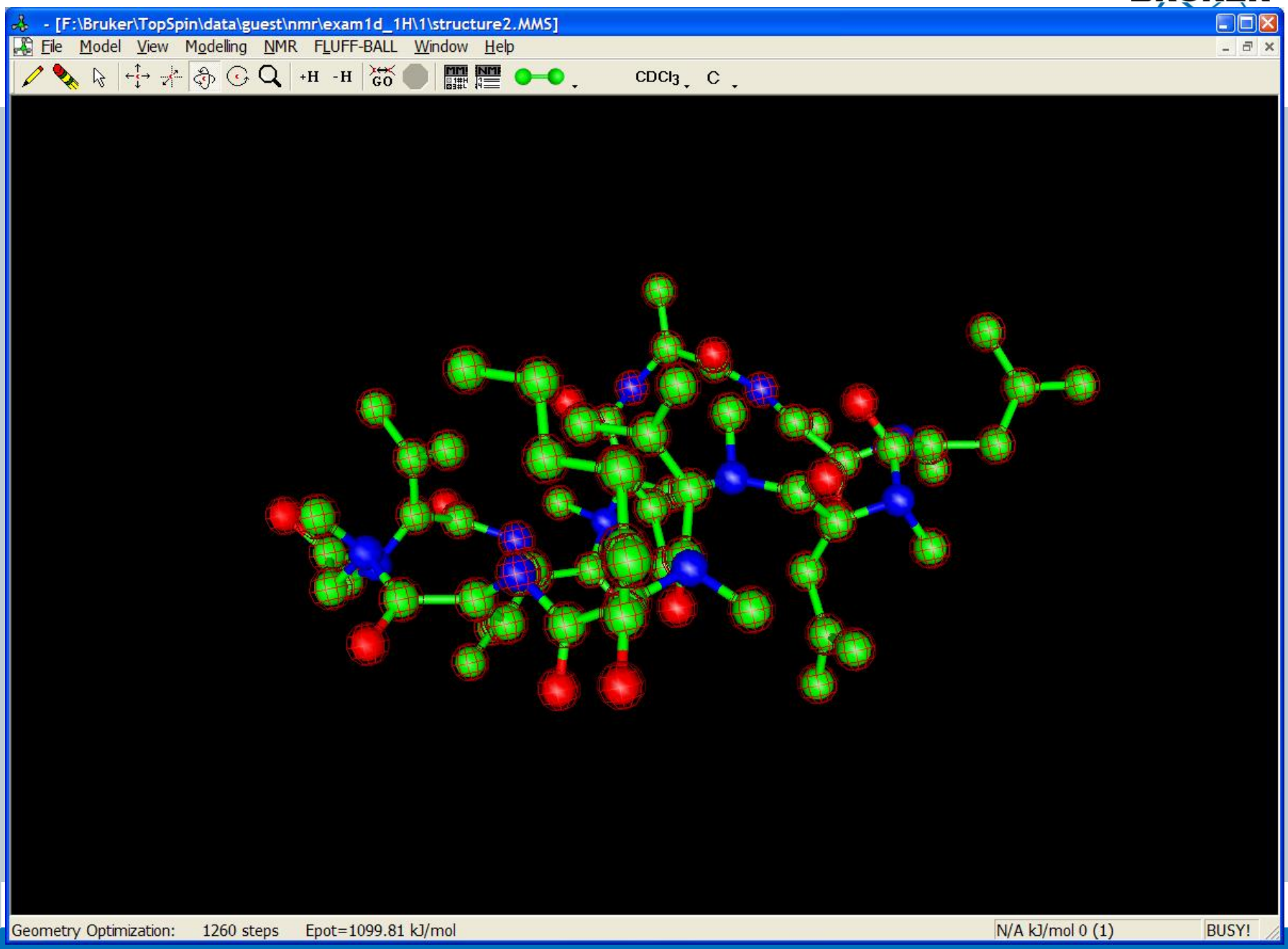




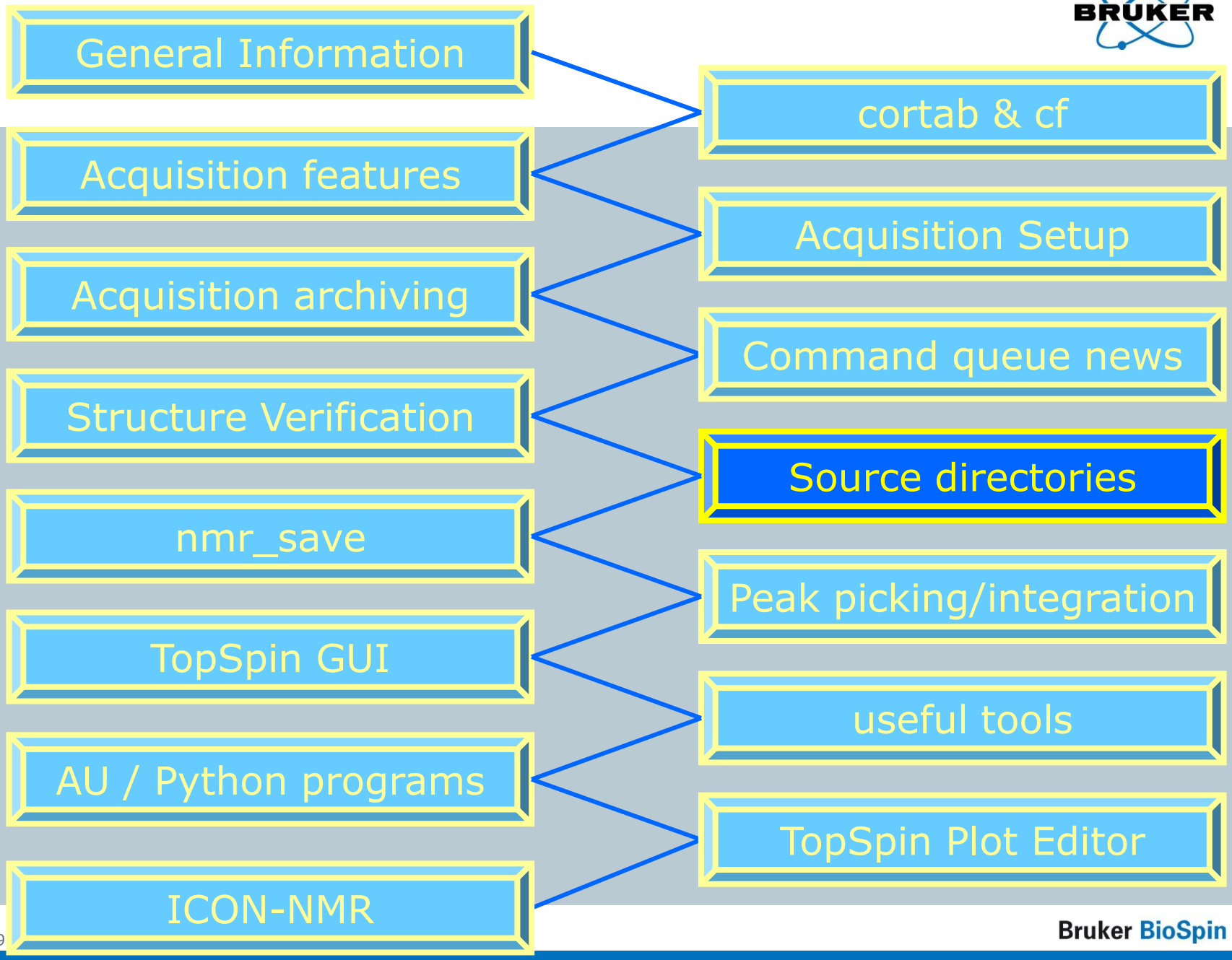


*Perch requires a separate license

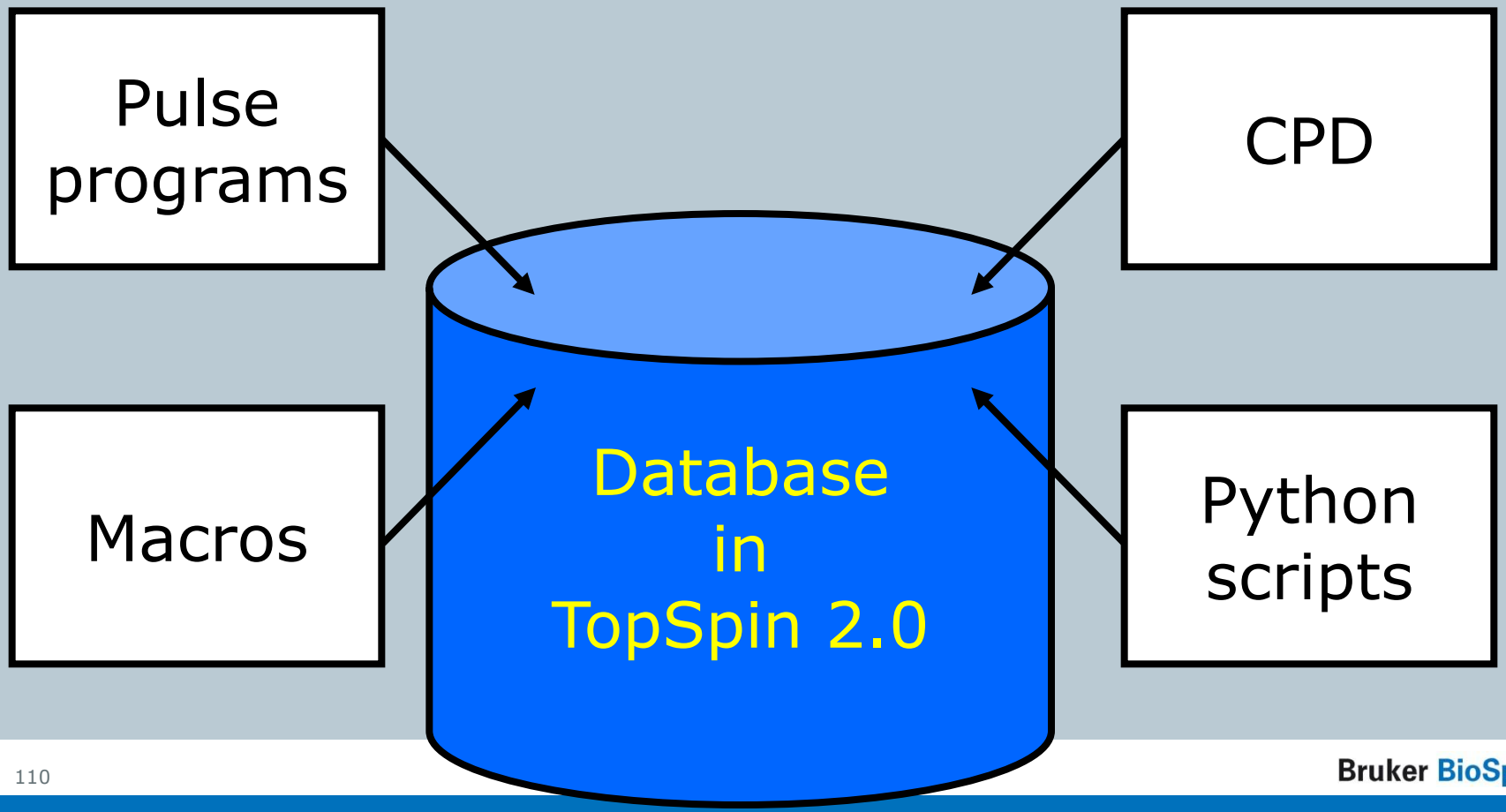
Perch*: e.g. geometry optimization



Content

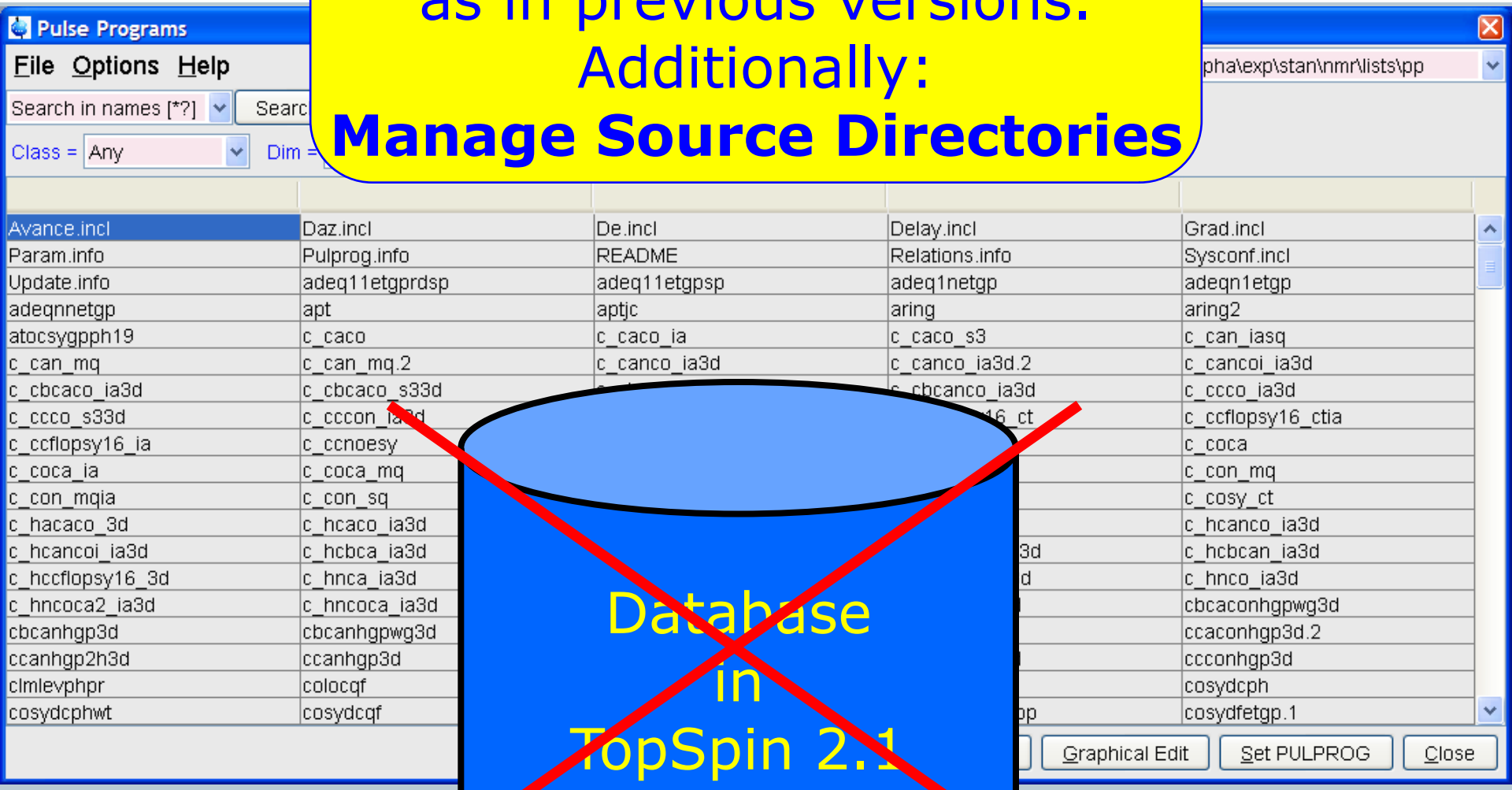

General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

Pulse programs in TopSpin 2.0



e.g. **edpul**

No database anymore in 2.1!
Again directory/file structure
as in previous versions.
Additionally:
Manage Source Directories



e.g. **edpul**

No database anymore in 2.1!
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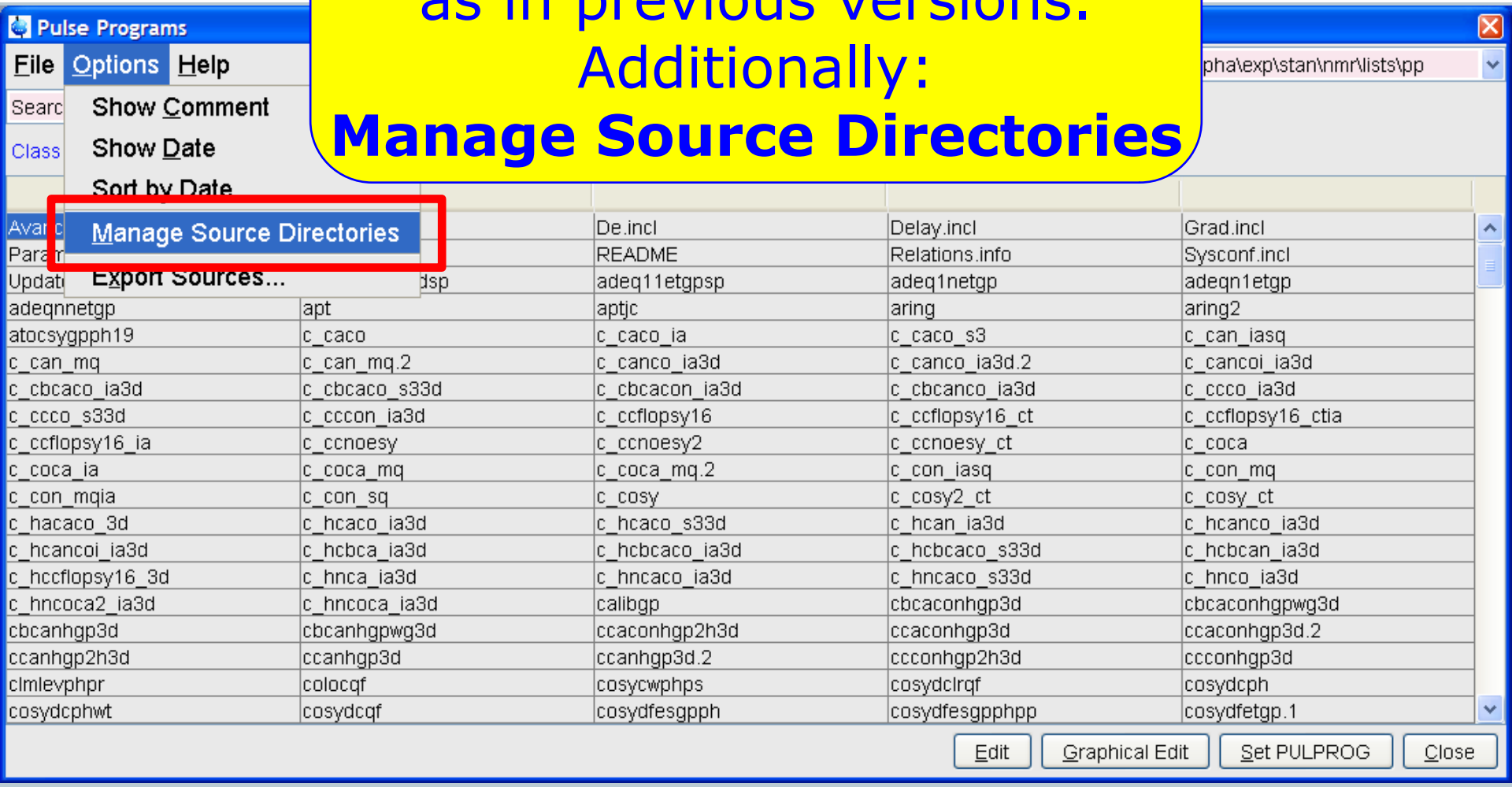
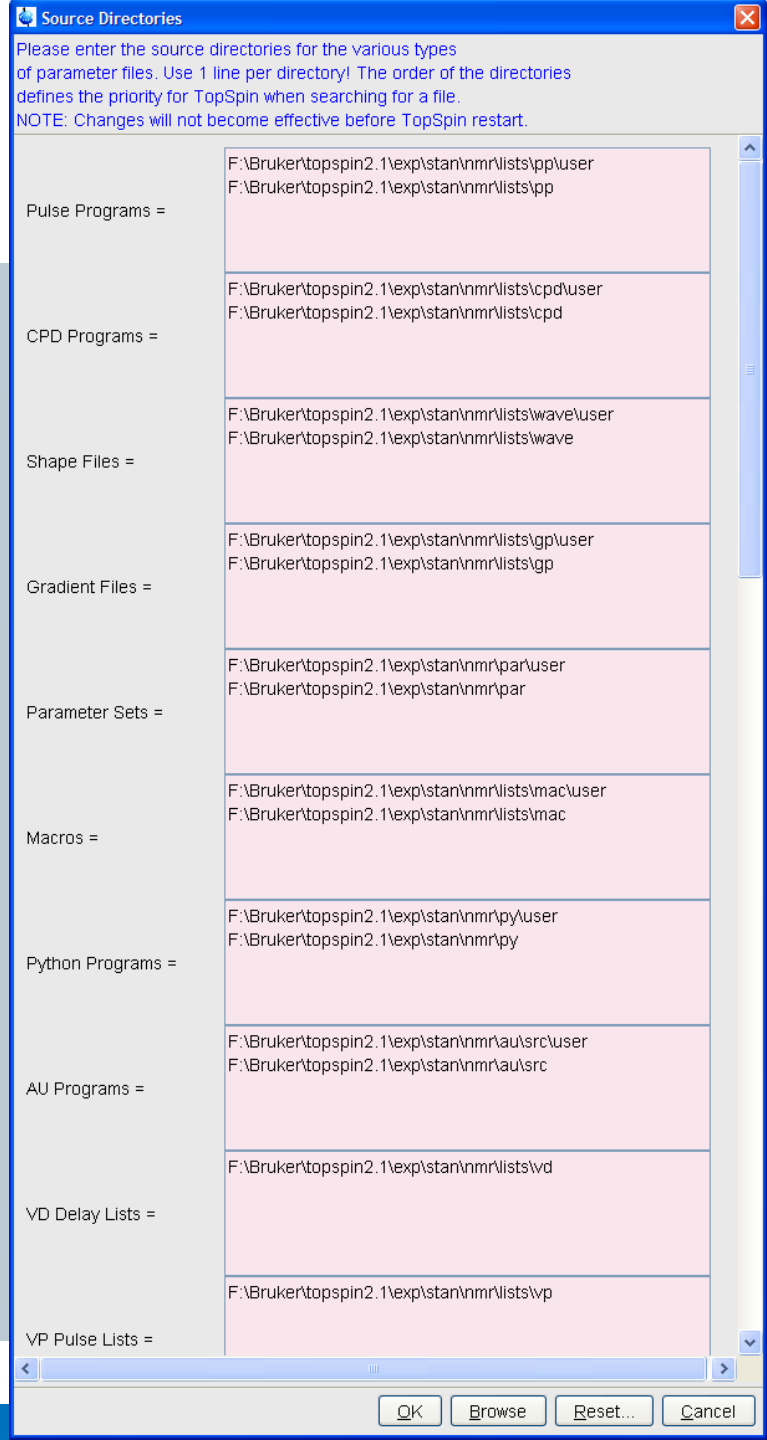


Source directories

User can specify individual directories for:

- Pulse programs
- CPD programs
- Shape Files
- Gradient Files
- Parameter Sets
- Macros
- Python programs
- AU programs
- VD lists
- VP lists …

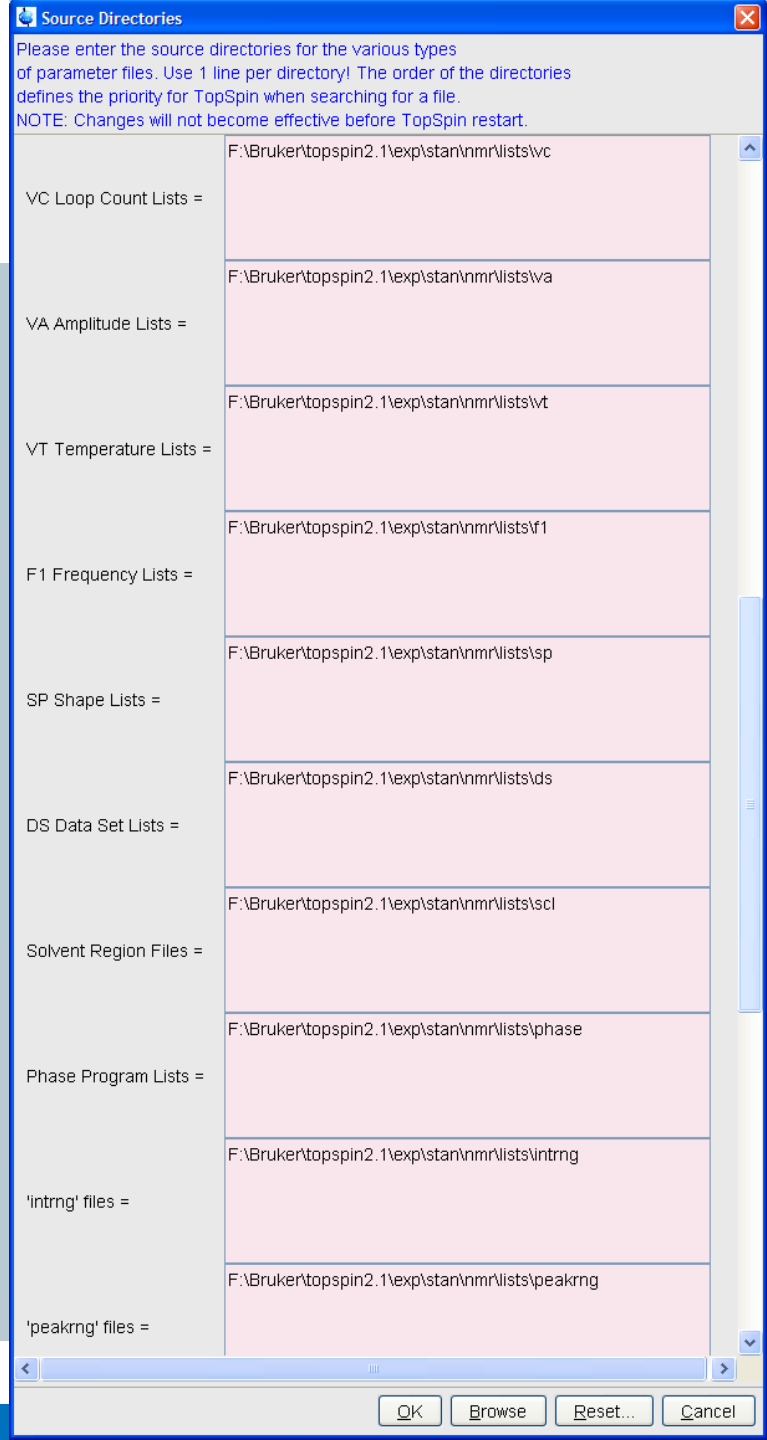


Source directories

User can specify individual directories for:

…

- VC lists
- VA lists
- VT lists
- F1 lists
- SP lists
- DS lists
- Solvent Region Files
- Phase lists
- intrng files …



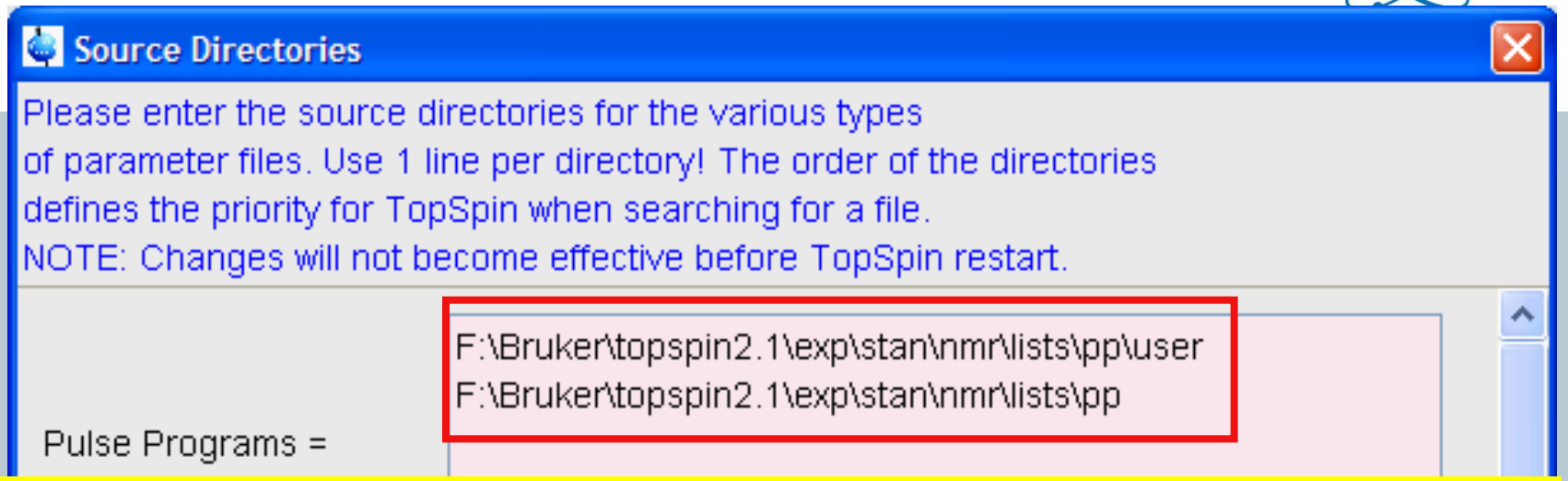
Source directories

User can specify individual directories for:

...

- peakrng files
- baslpnts files
- base_info files
- peaklist files
- clevels files
- reg files
- int2drng files
- structure files

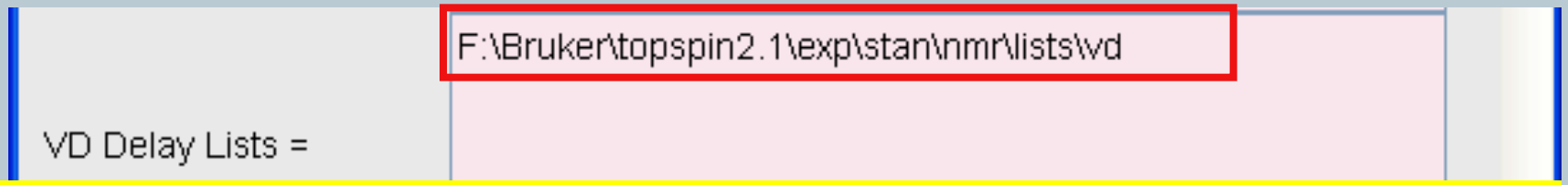
Default directories



Default path for e.g. pulse programs:

Bruker files in: *.../exp/stan/nmr/lists/pp*

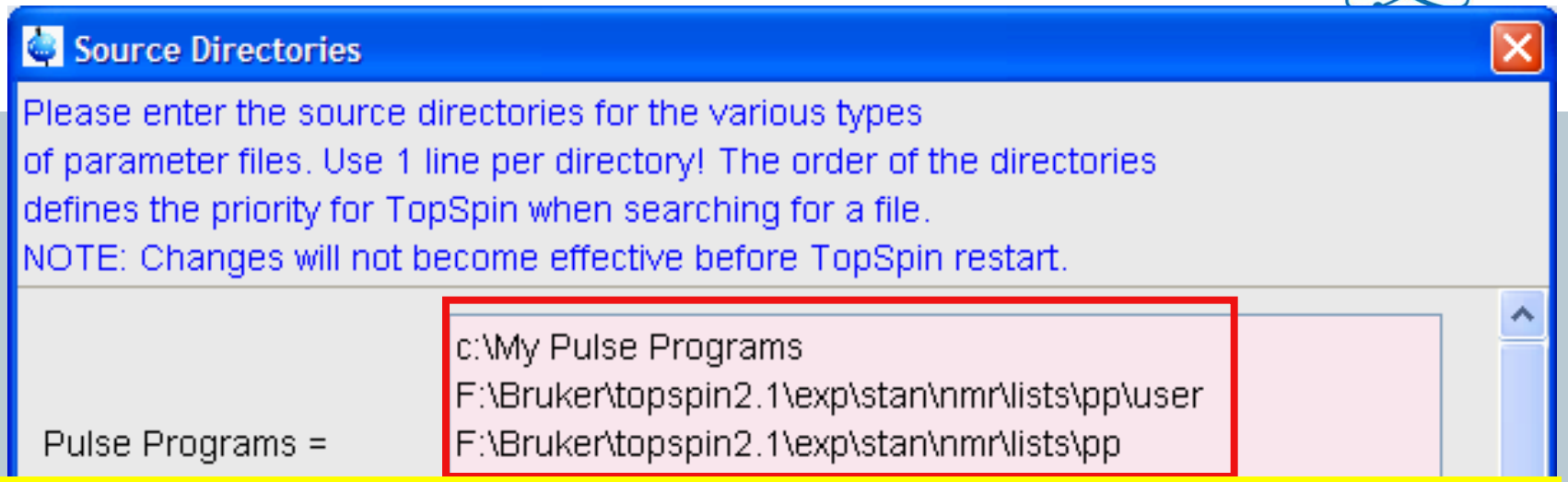
User files in: *.../exp/stan/nmr/lists/pp/user*



Default path for e.g. VD lists:

Bruker/User files in: *.../exp/stan/nmr/lists/vd*

Default directories



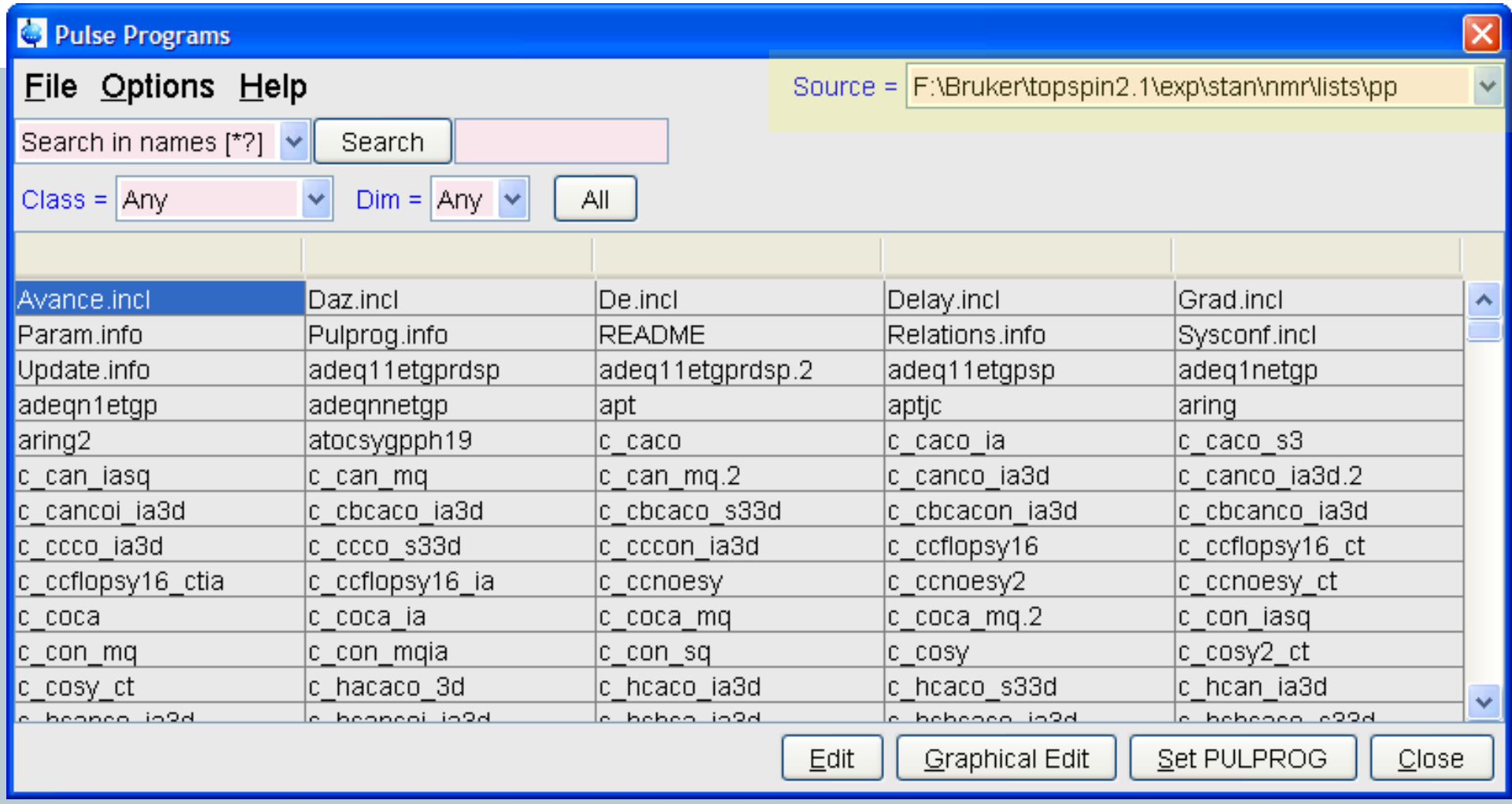
Default path for pulse programs:

Bruker files in: *.../exp/stan/nmr/lists/pp*

User files in: *.../exp/stan/nmr/lists/pp/user*

Each user can define his own directories
(in an unlimited number)

Definition of the content of e.g.: **edpul**



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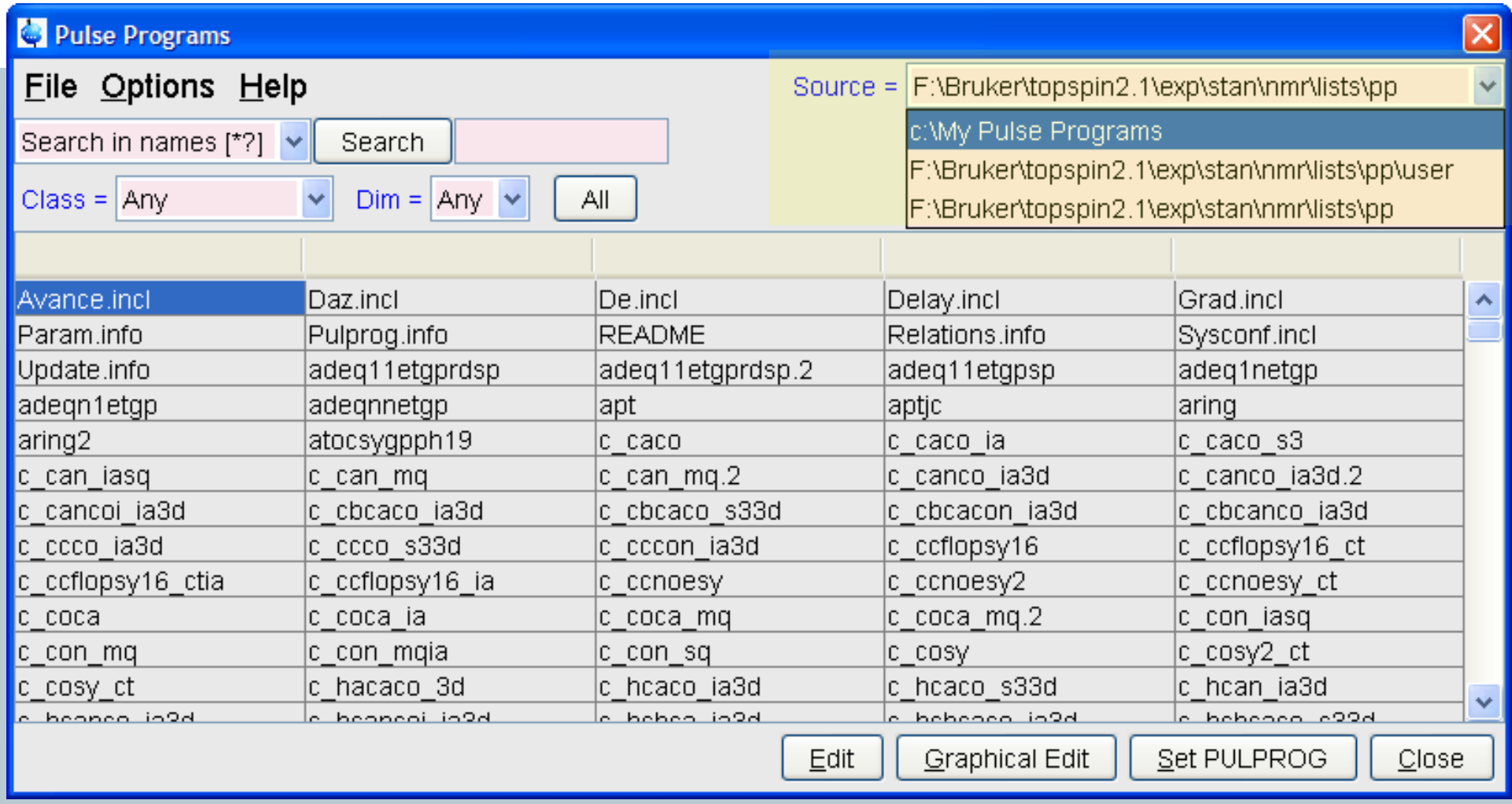
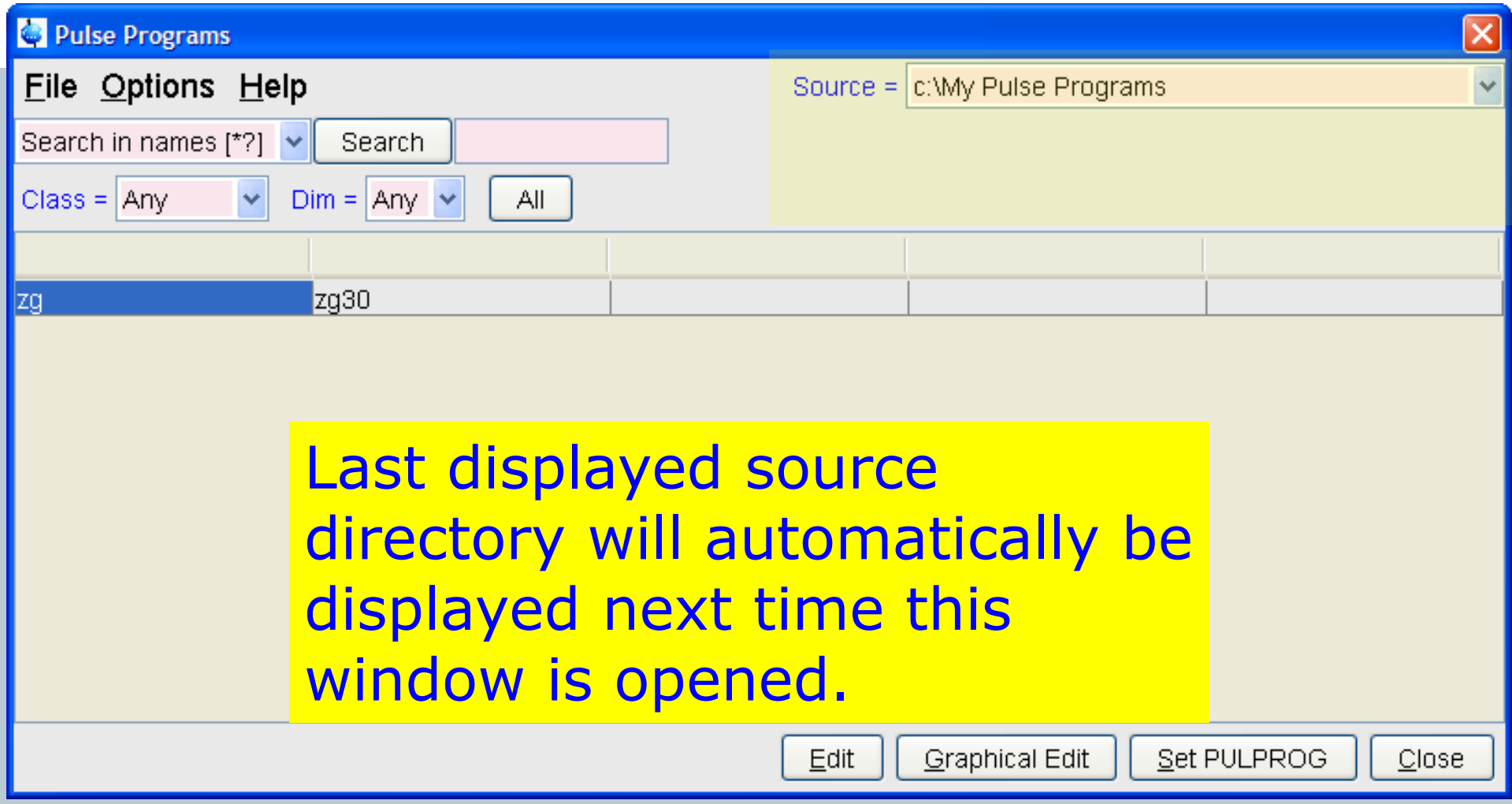
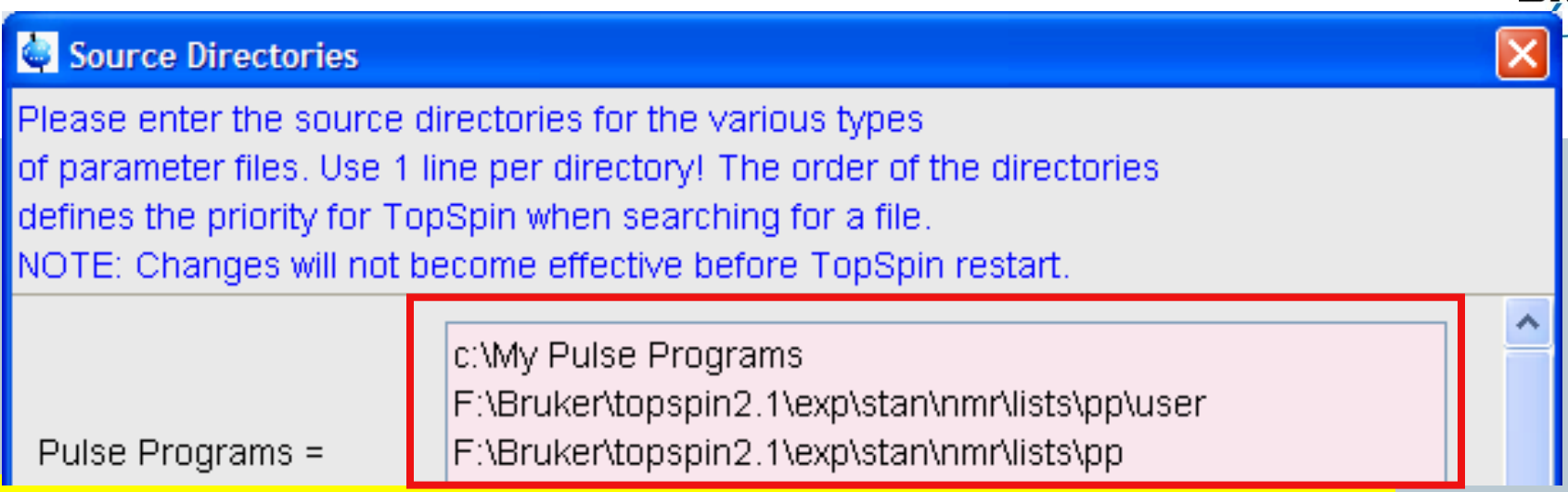


Definition of the content of e.g.: **edpul**



User-specific directory

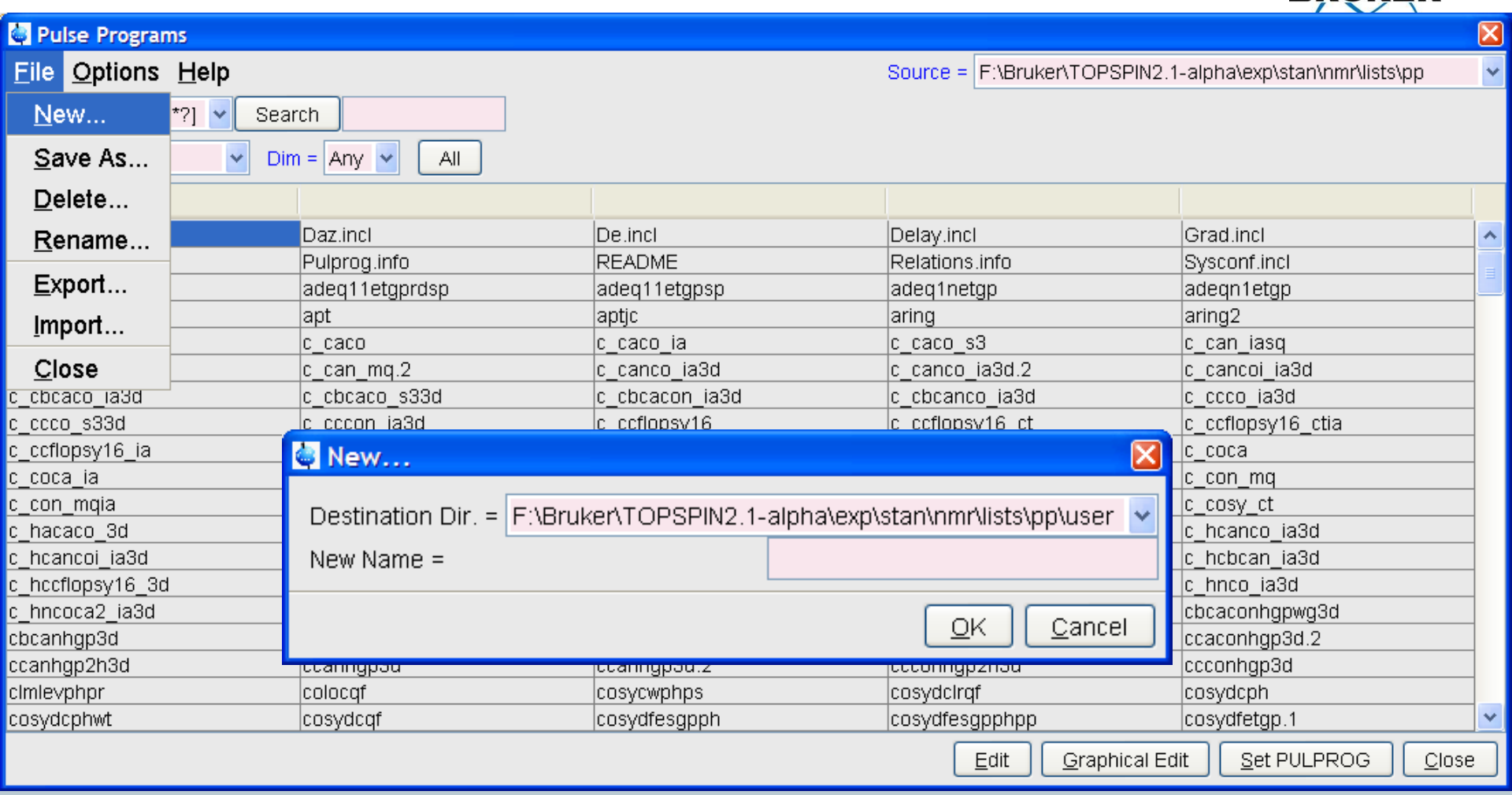


The order of the directories defines the priority for searching a file.

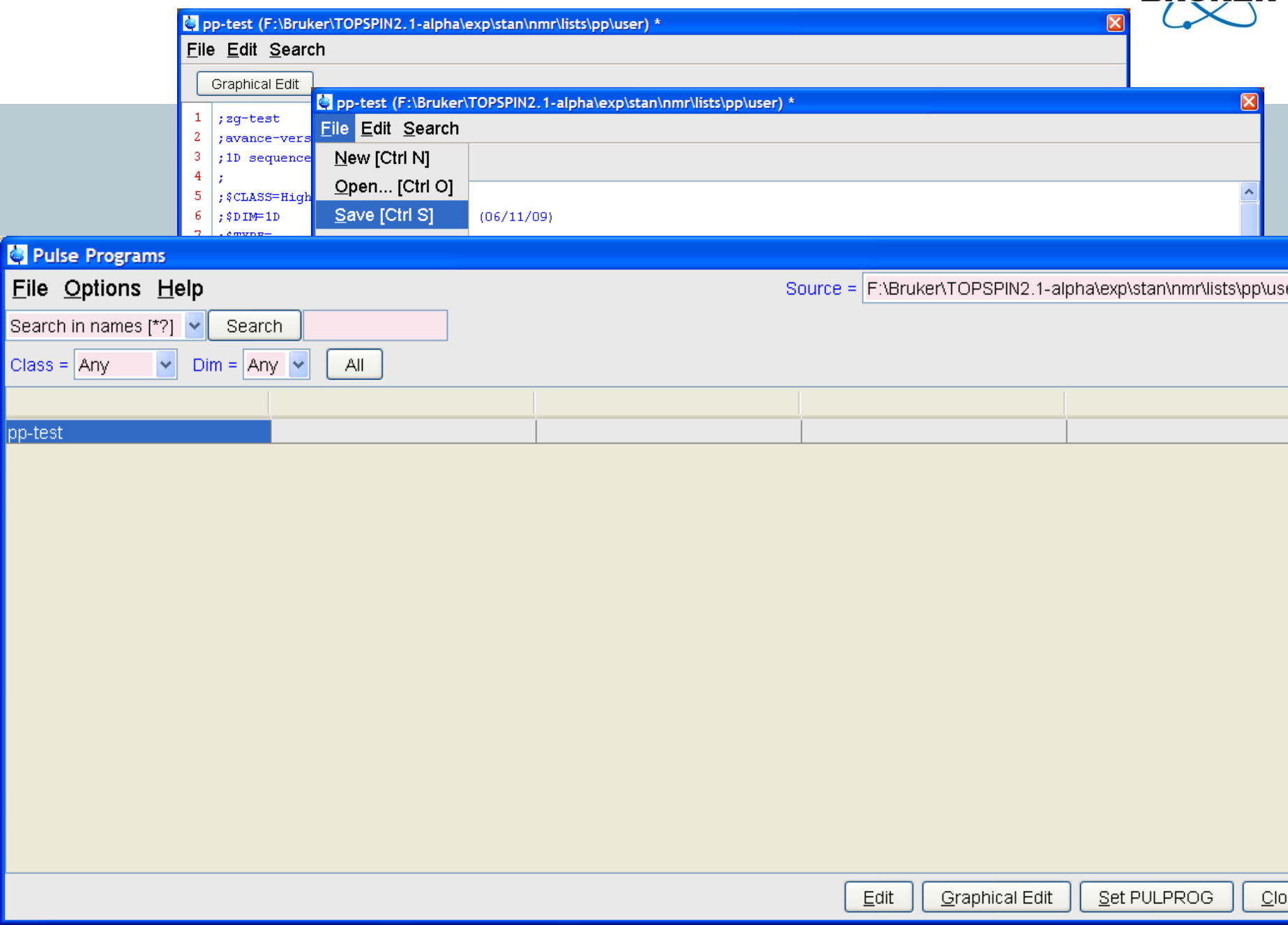
Example above:

1) Pulse program **zg** can be available in all three directories
2) e.g. **zg** should be used for acquisition,
   - ➔ TopSpin (and/or ICON-NMR) searches for **zg**
   - ➔ if the first directory *C:\My Pulse Programs* contains a **zg**
   - ➔ this one will be used for acquisition ('first come, first served')

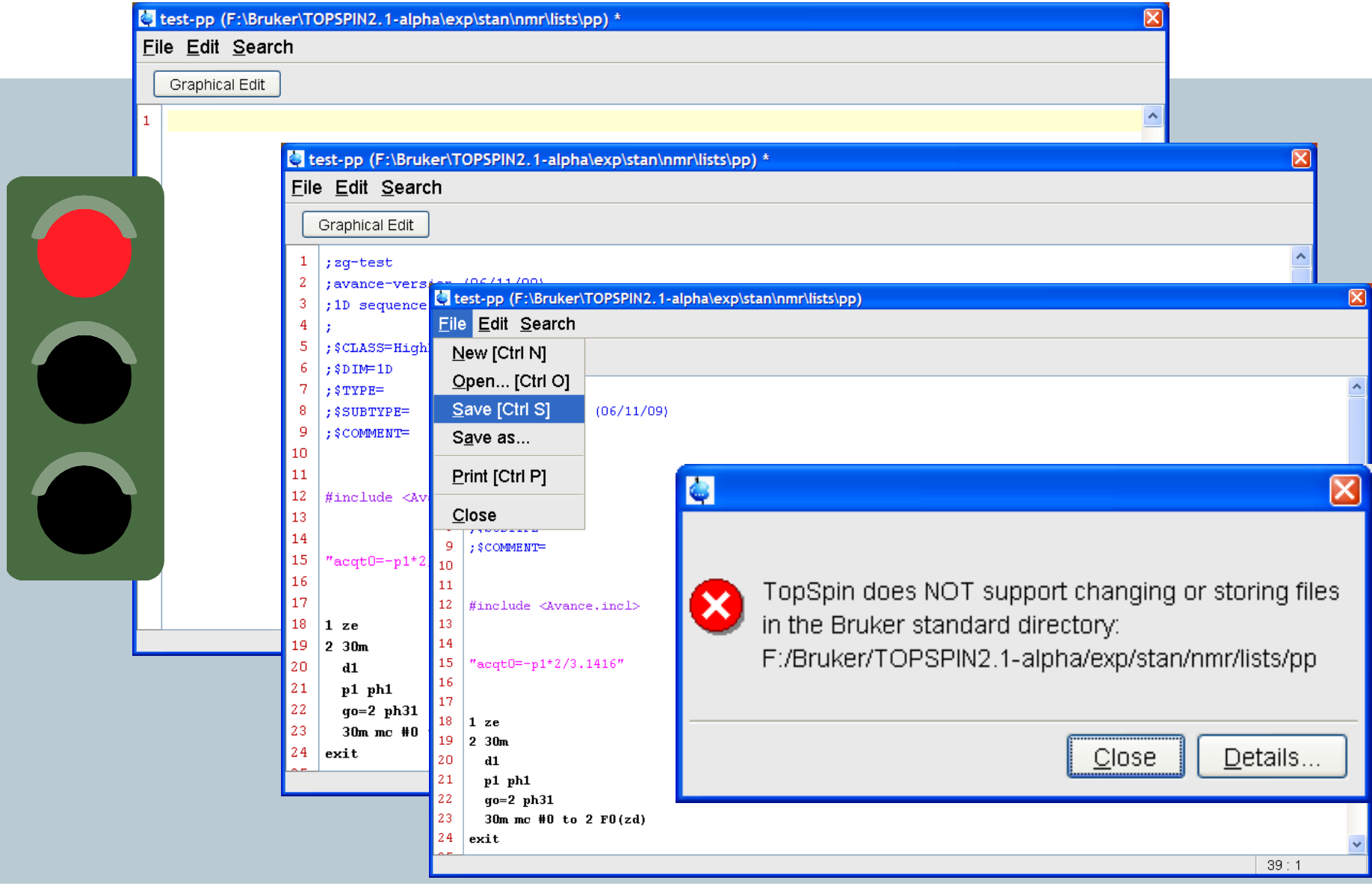
Create a new file in *pp/user* !



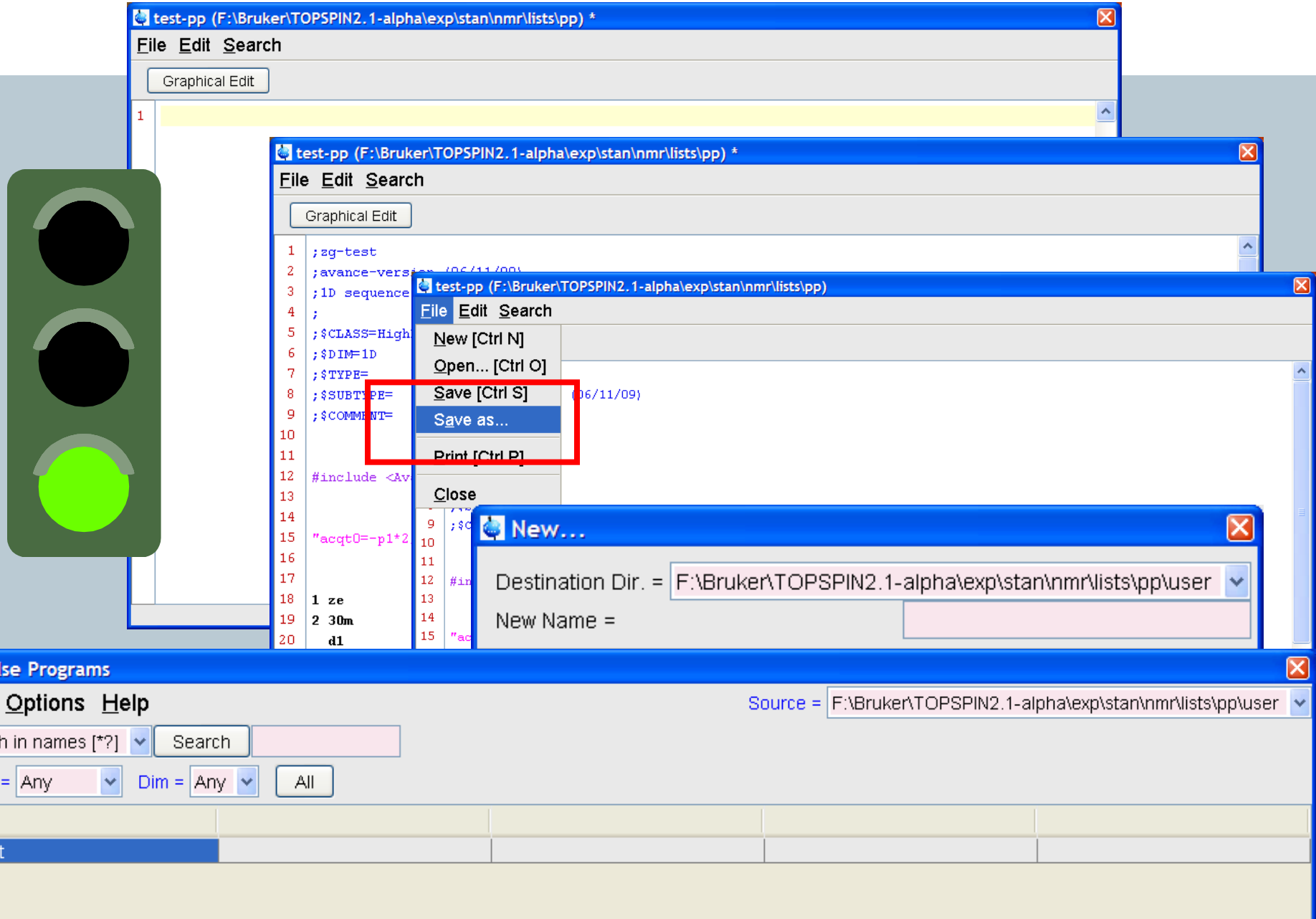
Create a new file in *pp/user* !



Create a new file in *pp* ?



Create a new file in *pp/user* !



Summary

1. each user starts with a list of default directories (e.g. *lists/pp* and *lists/pp/user*)

2. only the **user** directory is writable

3. each user can remove one or more default directories from its list

4. each user can specify one or more additional source directories

5. each user can define the order of the directories which defines the search order within TopSpin

Source directories – advantages
e.g. pulse programs

Bruker files in: *…/exp/stan/nmr/lists/pp*
These files are write protected!

➔ You can be sure that these files always contain the right content

User files in: *…/exp/stan/nmr/lists/pp/user*
By default any user-specific file will be stored here, they are read- and writable

➔ You have an easy setup to distribute user-specific files to all users of the spectrometer

Source directories – advantages
e.g. pulse programs

Each user can define his **own source directories**

➔ These files will have the permissions you want to!
If you store them e.g. in your home directory, the files will be only readable by yourself

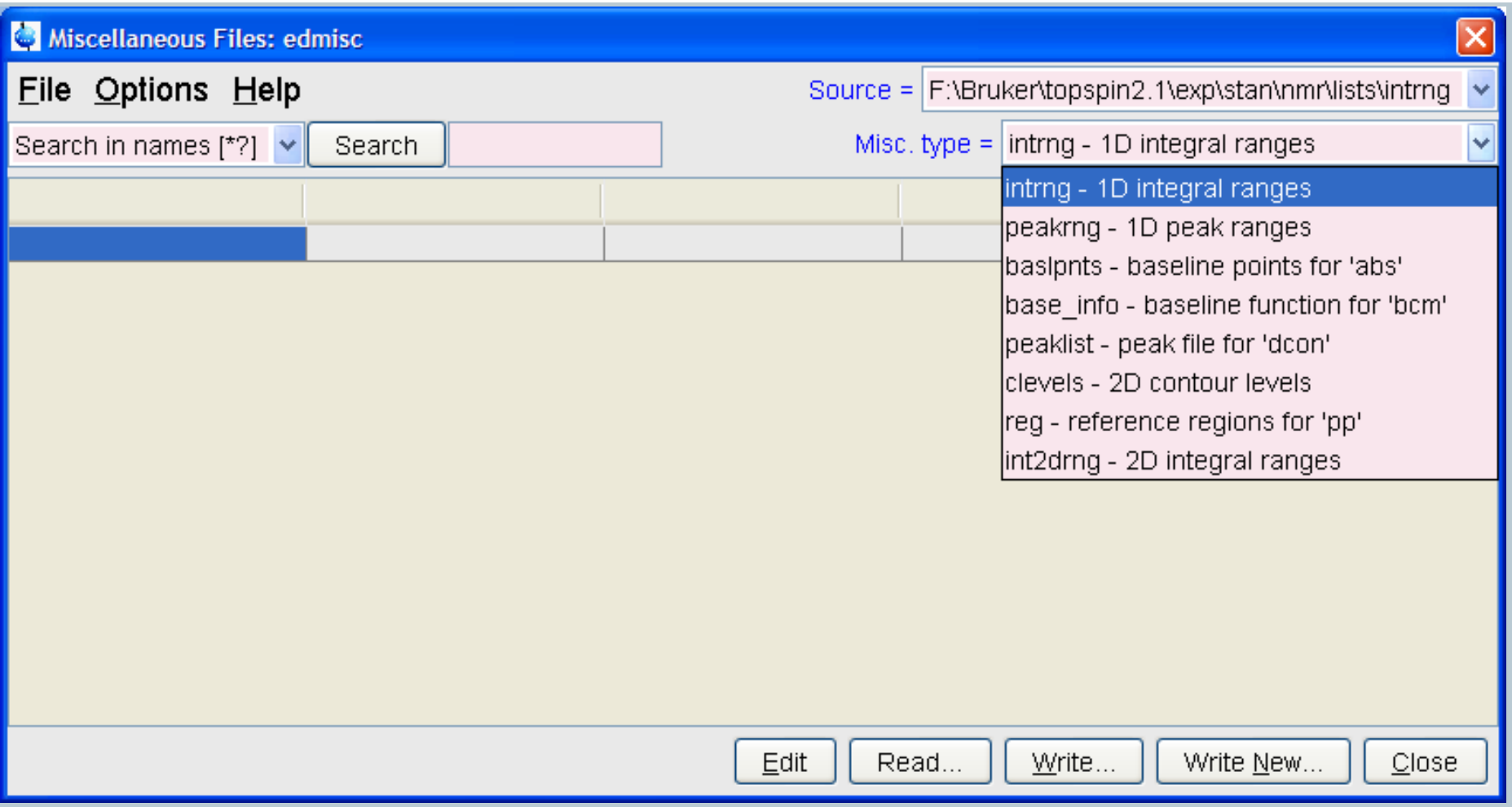
➔ These files can be easily distributed!
If you want to use e.g. your pulse programs on different spectrometers, just define a network drive as a source directory.

GUI available for …

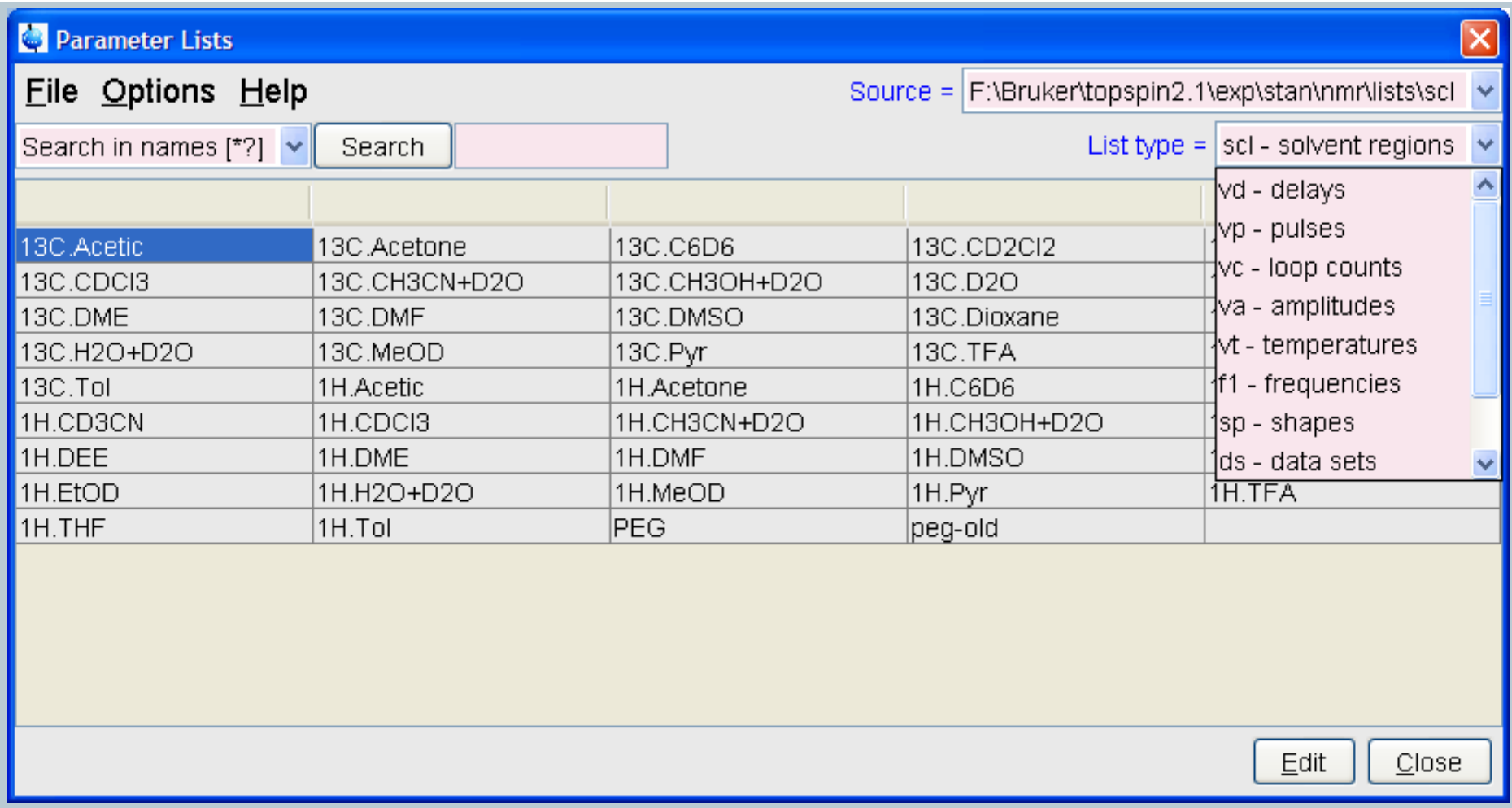
User can specify individual directories for:

- Pulse programs ➟ edpul
- CPD programs ➟ edcpd
- Shape Files ➟ edshape
- Parameter Sets ➟ rpar
- Macros ➟ edmac
- Python programs ➟ edpy
- AU programs ➟ edau
- VD,VP,VC,VA,VT,F1,DS, solvent region files, phases ➟ edlist
- intrng, peakrng, … ➟ edmisc

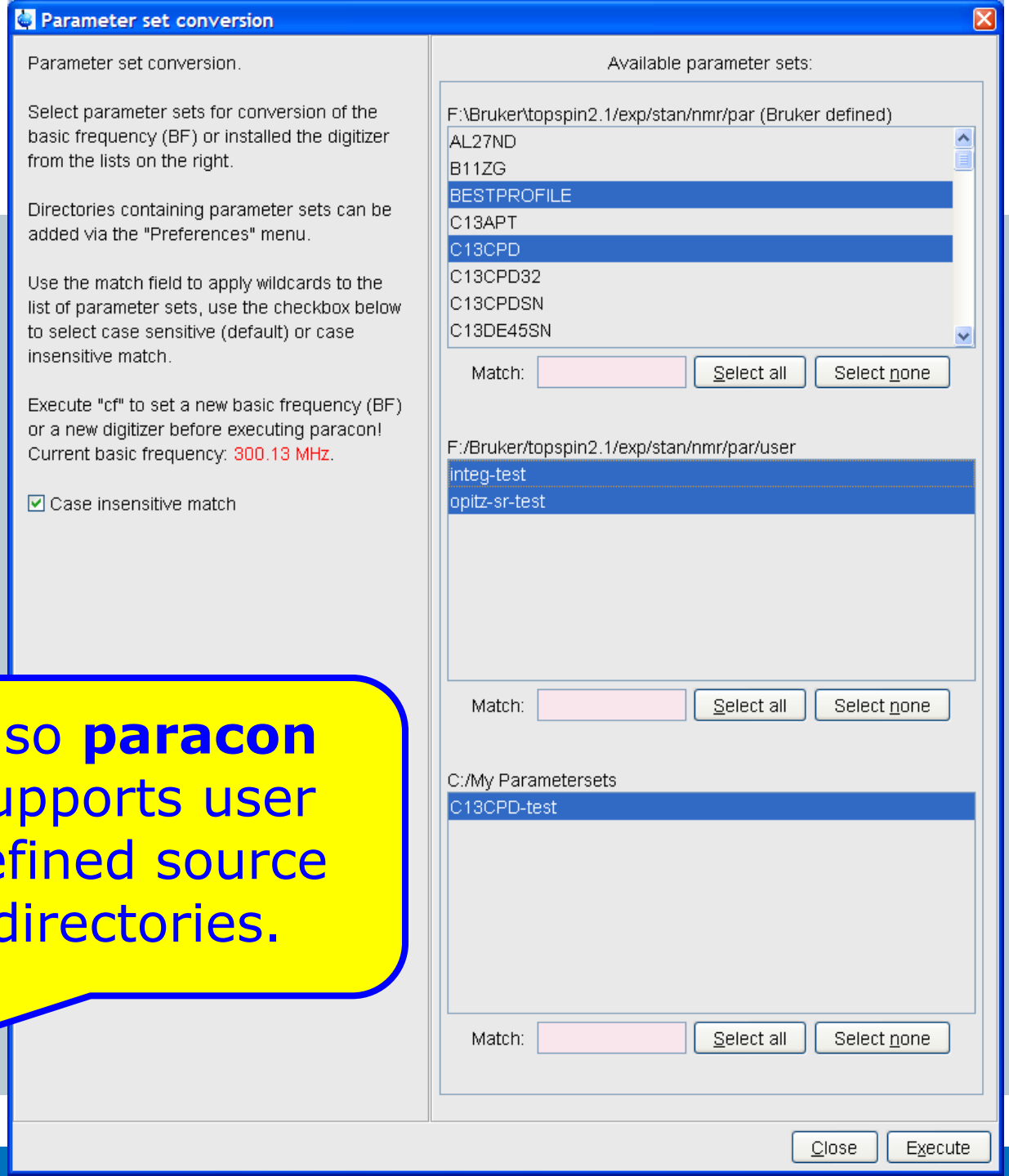
edmisc


Miscellaneous Files: edmisc
File Options Help
Source = F:\Bruker\topspin2.1\exp\stan\nmr\lists\intrng
Search in names [*?]
Search
Misc. type = intrng - 1D integral ranges
intrng - 1D integral ranges
peakrng - 1D peak ranges
baslpnts - baseline points for 'abs'
base_info - baseline function for 'bcm'
peaklist - peak file for 'dcon'
clevels - 2D contour levels
reg - reference regions for 'pp'
int2drng - 2D integral ranges
Edit
Read...
Write...
Write New...
Close

edlist

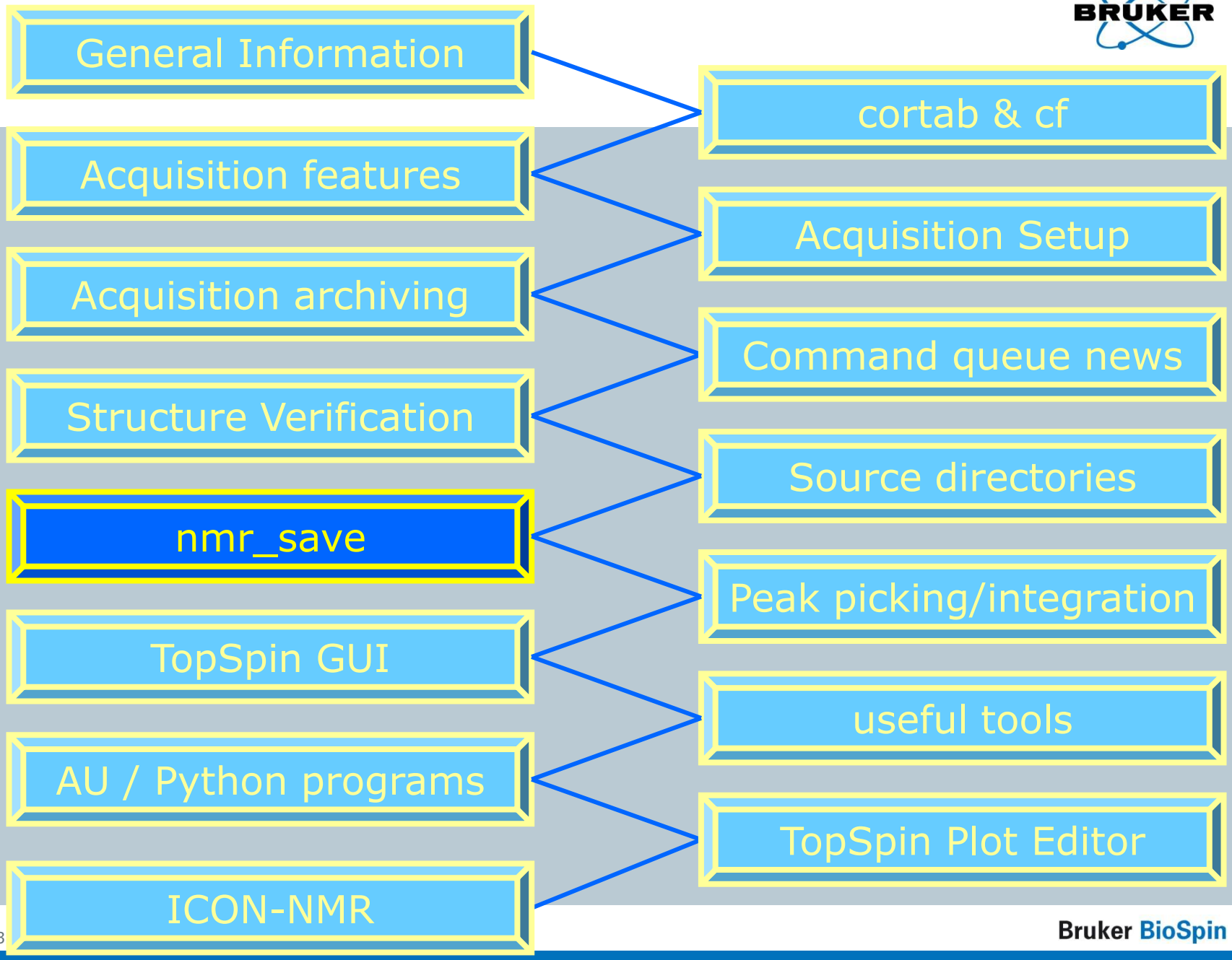

Parameter Lists
File Options Help
Source = F:\Bruker\topspin2.1\exp\stan\nmr\lists\scl
Search in names [*?]
Search
List type = scl - solvent regions
vd - delays
vp - pulses
vc - loop counts
va - amplitudes
vt - temperatures
f1 - frequencies
sp - shapes
ds - data sets
13C.Acetic
13C.Acetone
13C.C6D6
13C.CD2Cl2
13C.CDCl3
13C.CH3CN+D2O
13C.CH3OH+D2O
13C.D2O
13C.DME
13C.DMF
13C.DMSO
13C.Dioxane
13C.H2O+D2O
13C.MeOD
13C.Pyr
13C.TFA
13C.Tol
1H.Acetic
1H.Acetone
1H.C6D6
1H.CD3CN
1H.CDCl3
1H.CH3CN+D2O
1H.CH3OH+D2O
1H.DEE
1H.DME
1H.DMF
1H.DMSO
1H.EtOD
1H.H2O+D2O
1H.MeOD
1H.Pyr
1H.TFA
1H.THF
1H.Tol
PEG
peg-old
Edit
Close

paracon

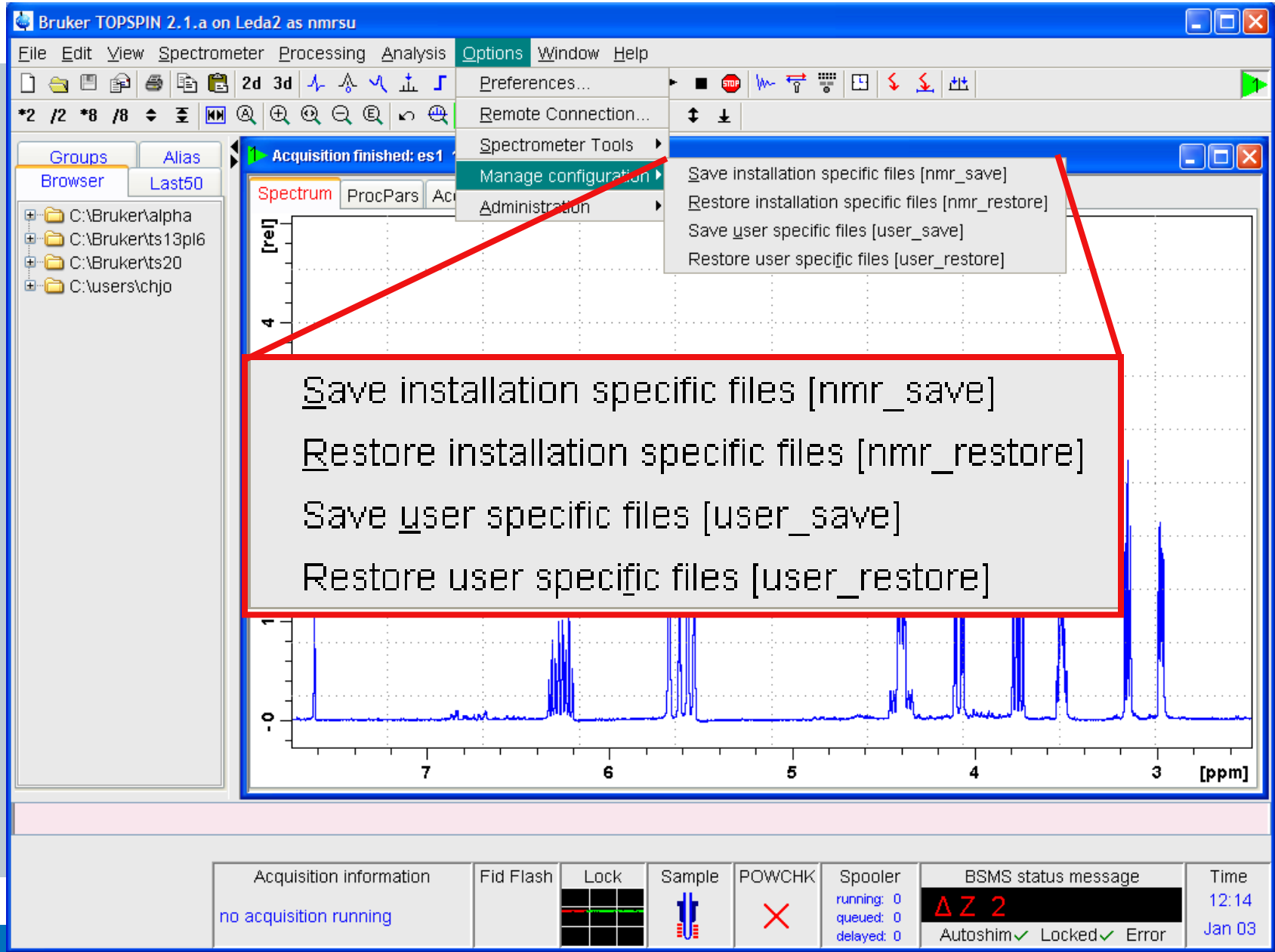


Also **paracon** supports user defined source directories.

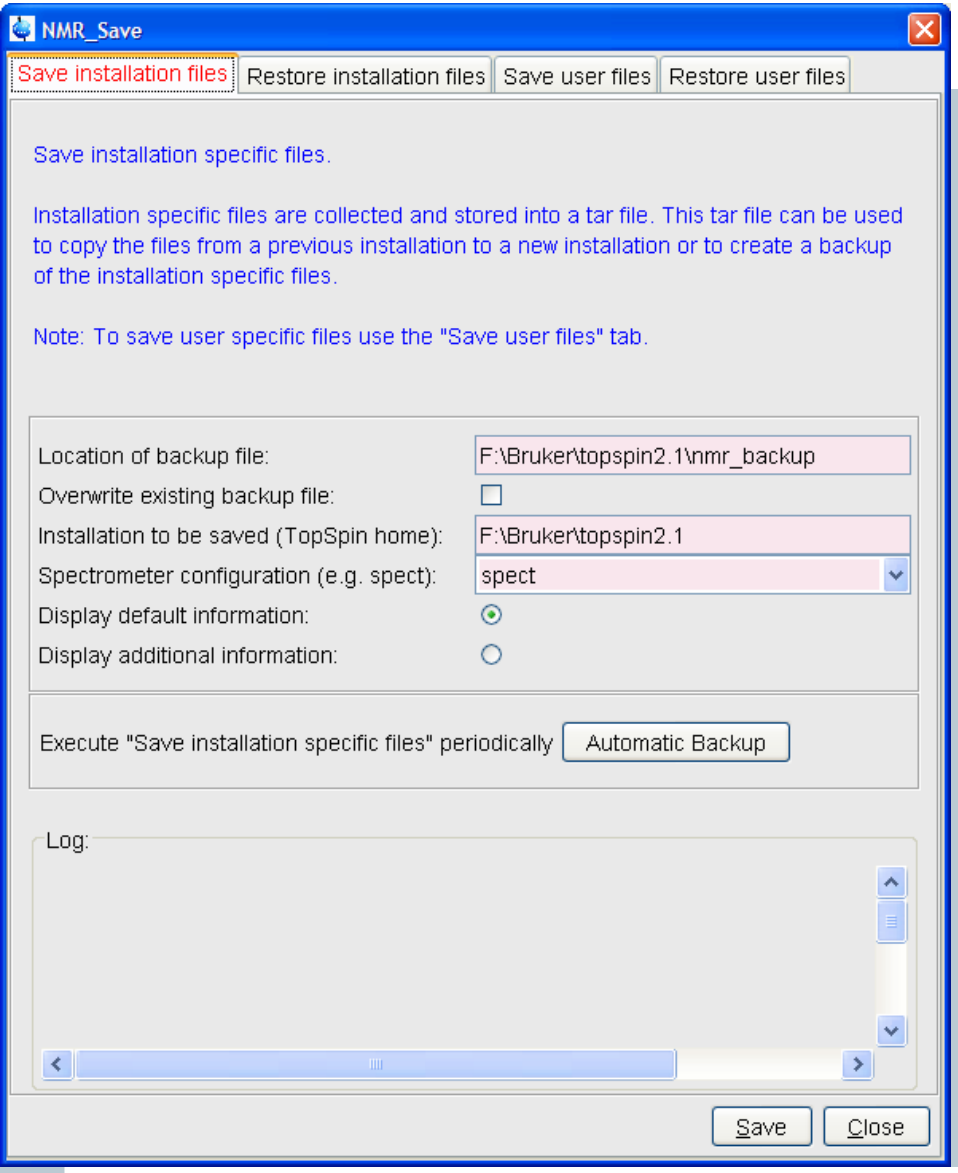
Content

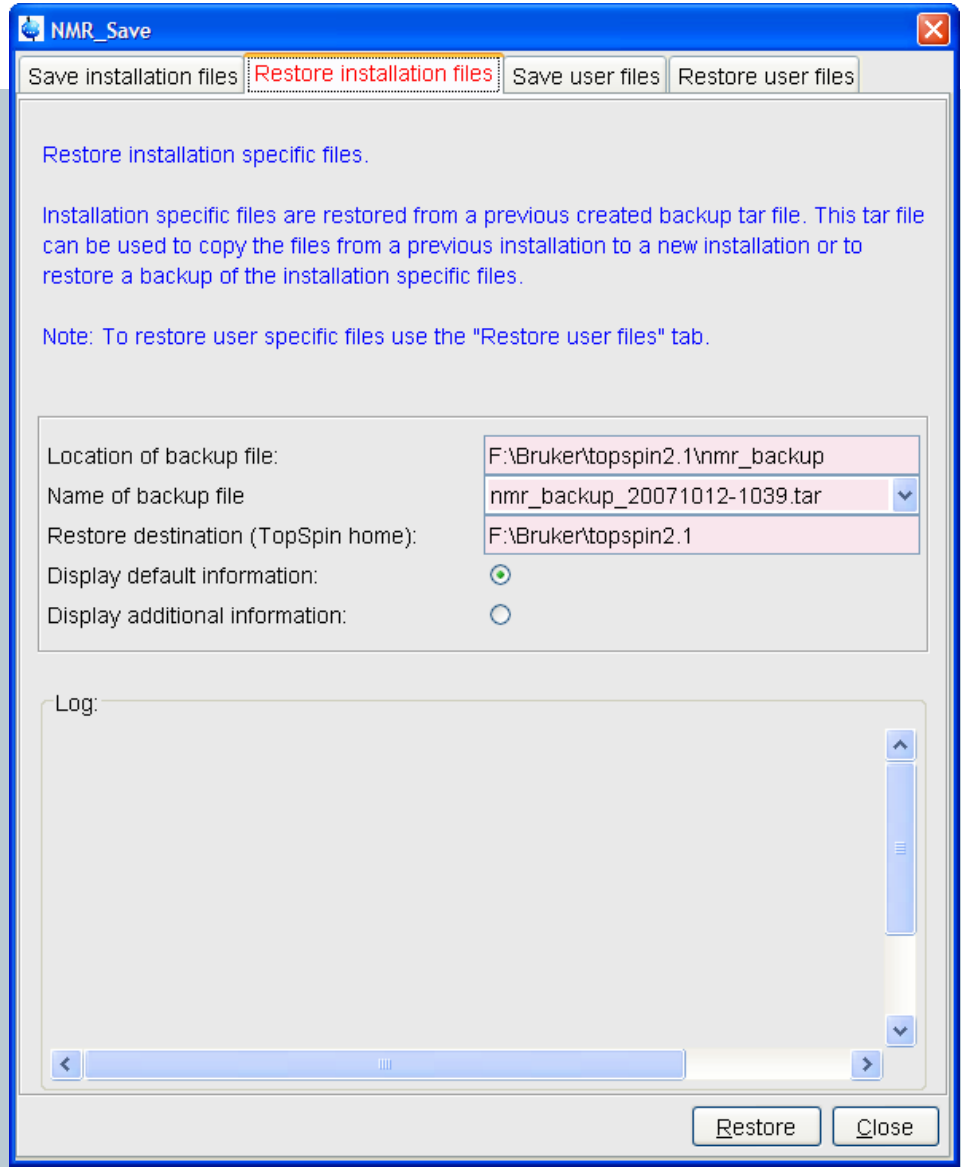

General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

nmr_save

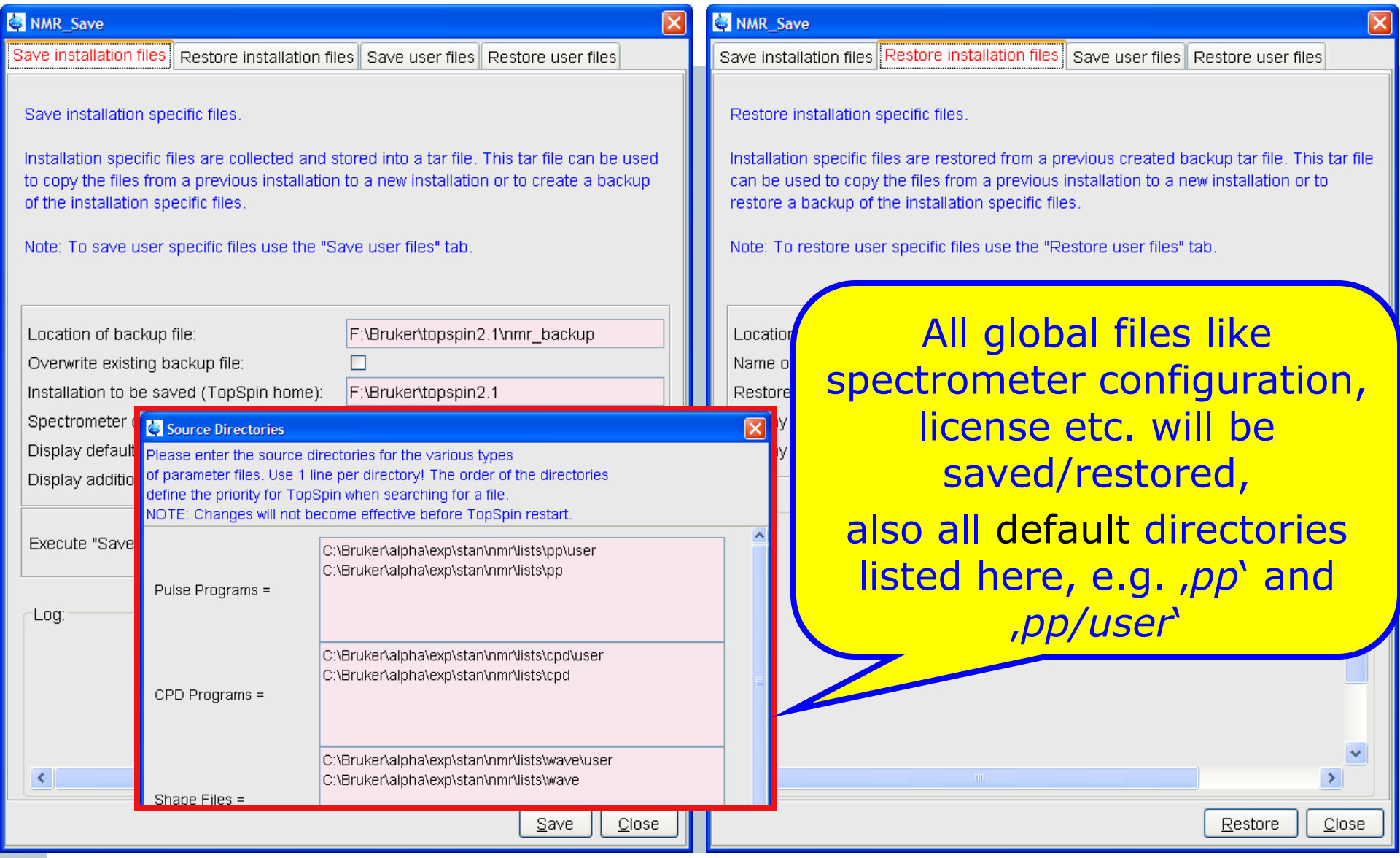

Bruker TOPSPIN 2.1.a on Leda2 as nmrsu
File Edit View Spectrometer Processing Analysis Options Window Help
Preferences...
Remote Connection...
Spectrometer Tools
Manage configuration
Administration
Save installation specific files [nmr_save]
Restore installation specific files [nmr_restore]
Save user specific files [user_save]
Restore user specific files [user_restore]
Groups
Alias
Browser
Last50
C:\Bruker\alpha
C:\Bruker\ts13pl6
C:\Bruker\ts20
C:\users\chjo
Acquisition finished: es1
Spectrum
ProcPars
[rel]
7
6
5
4
3
[ppm]
Acquisition information
no acquisition running
Fid Flash
Lock
Sample
POWCHK
Spooler
running: 0
queued: 0
delayed: 0
BSMS status message
Autoshim
Locked
Error
Time
12:14
Jan 03

nmr_save/restore





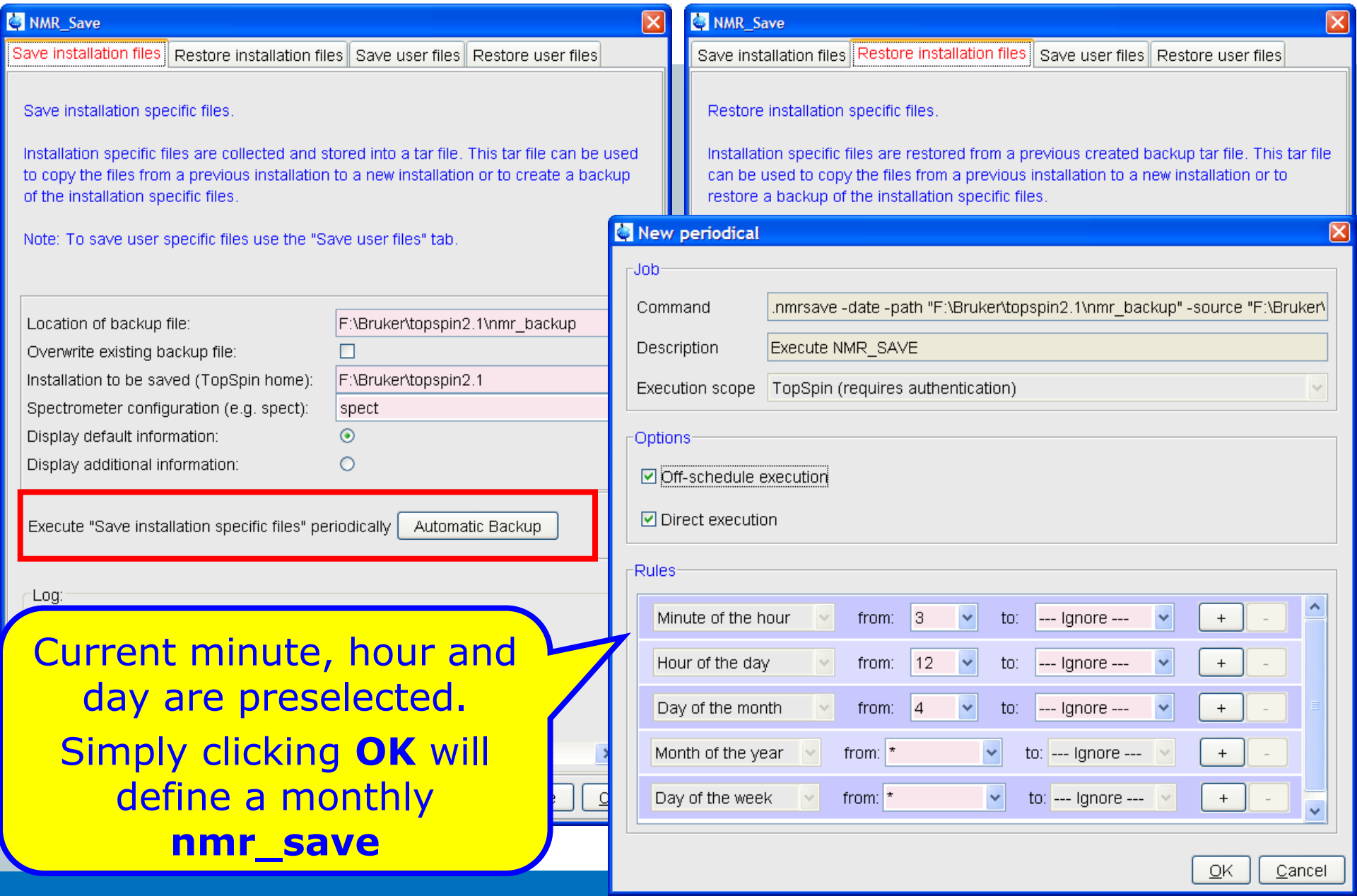
nmr_save/restore



All global files like spectrometer configuration, license etc. will be saved/restored,

also all default directories listed here, e.g. ‚*pp*' and ‚*pp/user*'

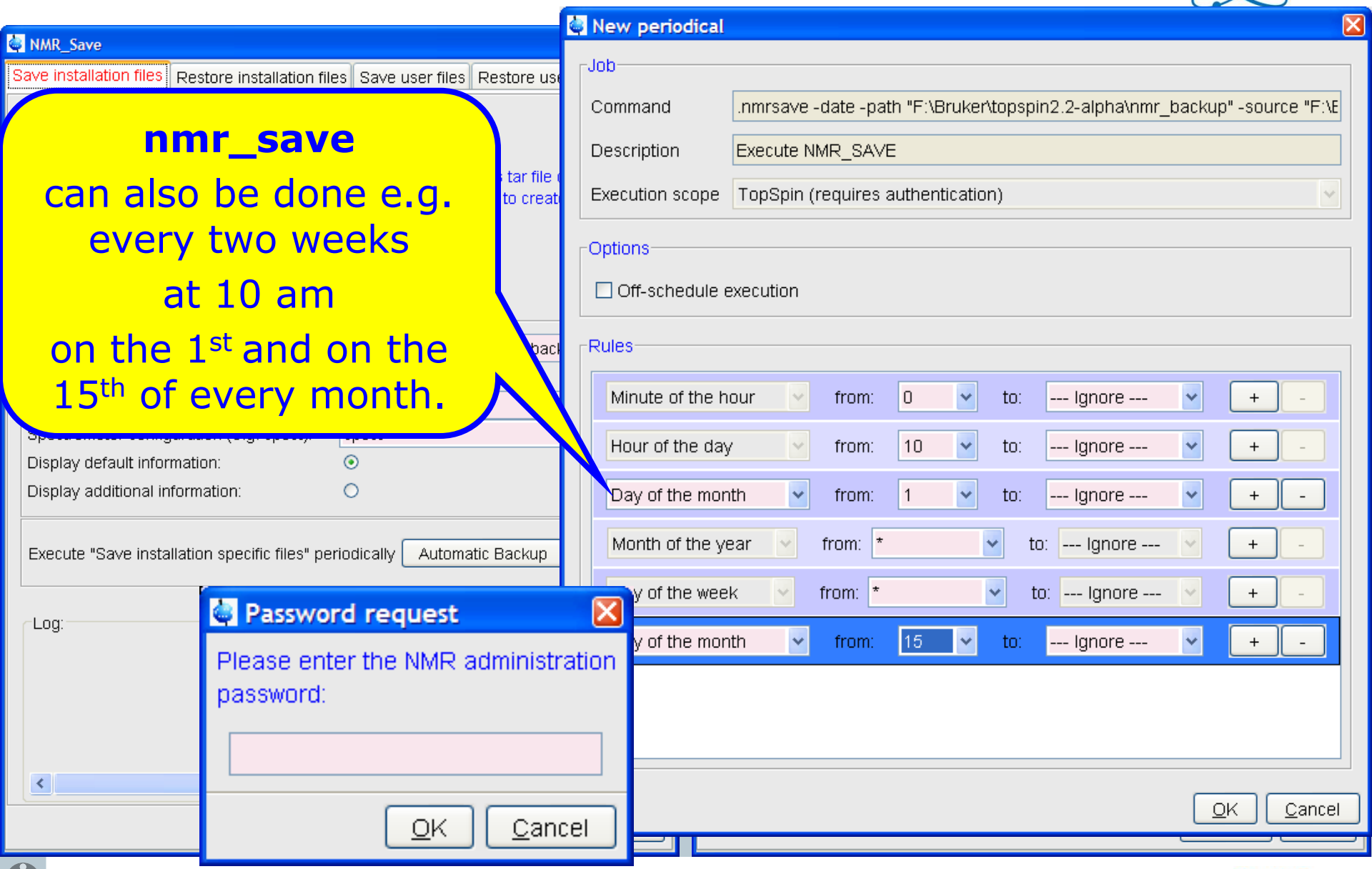
nmr_save/restore



Current minute, hour and day are preselected.

Simply clicking **OK** will define a monthly **nmr_save**

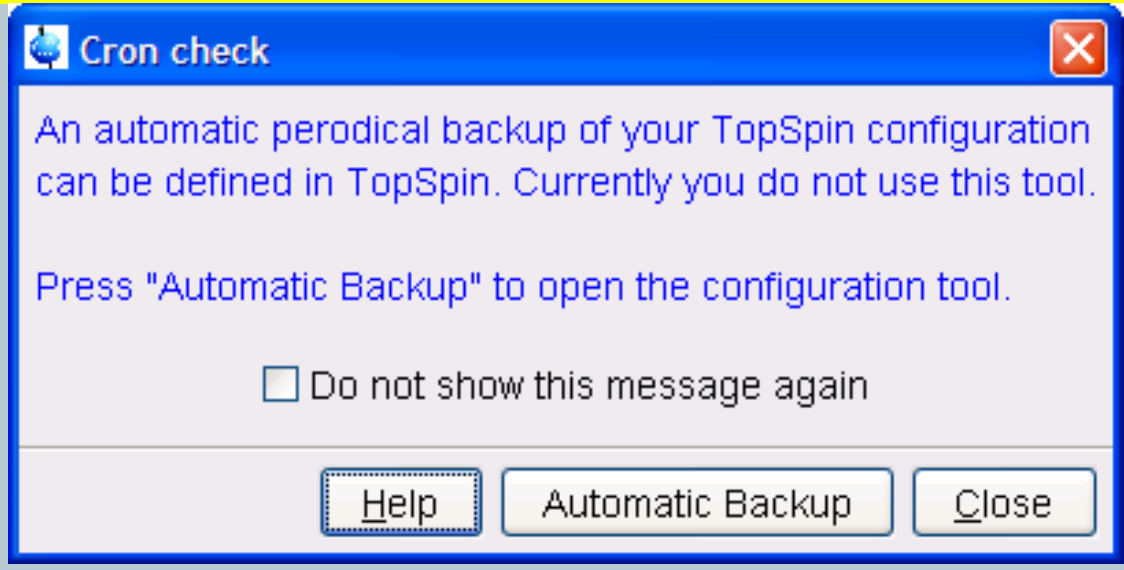
nmr_save/restore



nmr_save periodically

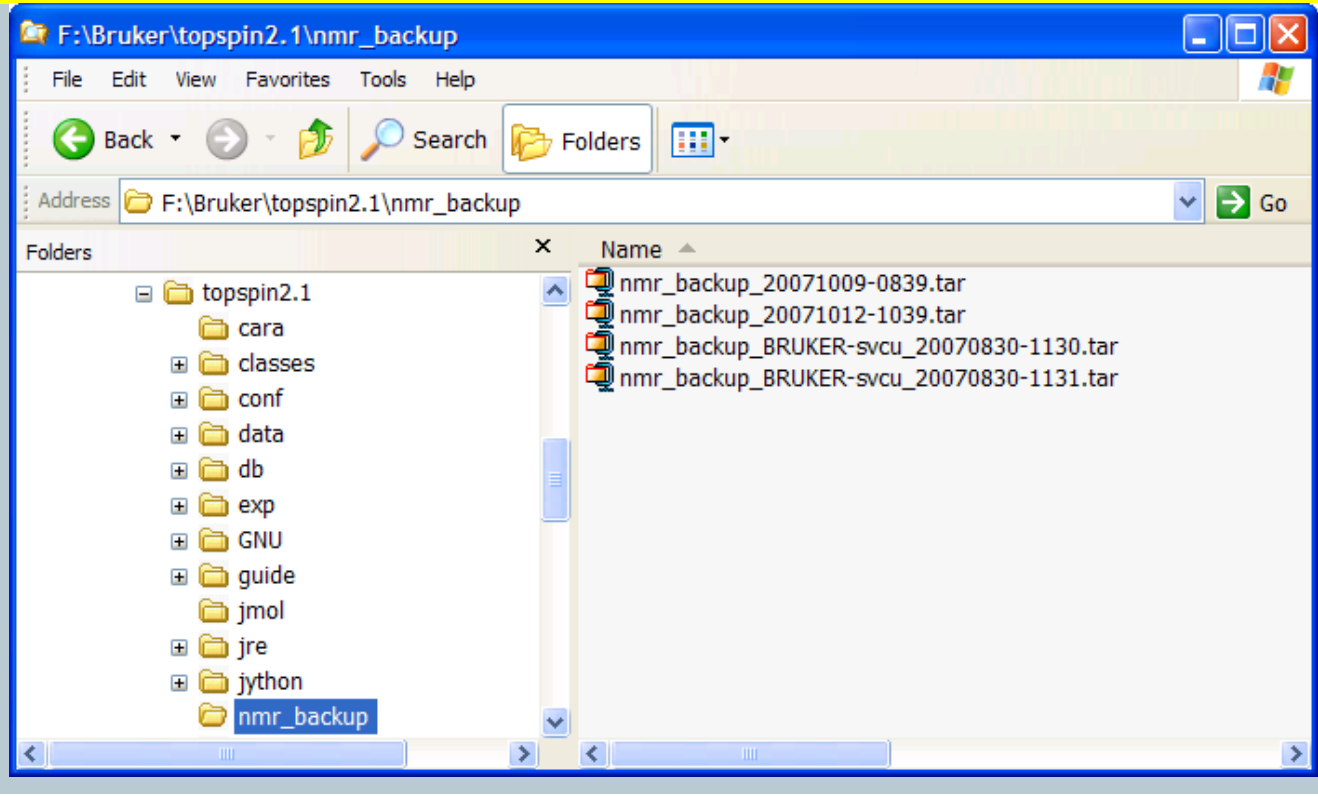
When **expinstall** is finished it is checked if an automatic periodic job for **nmr_save** exists.

If not, this message pops up:

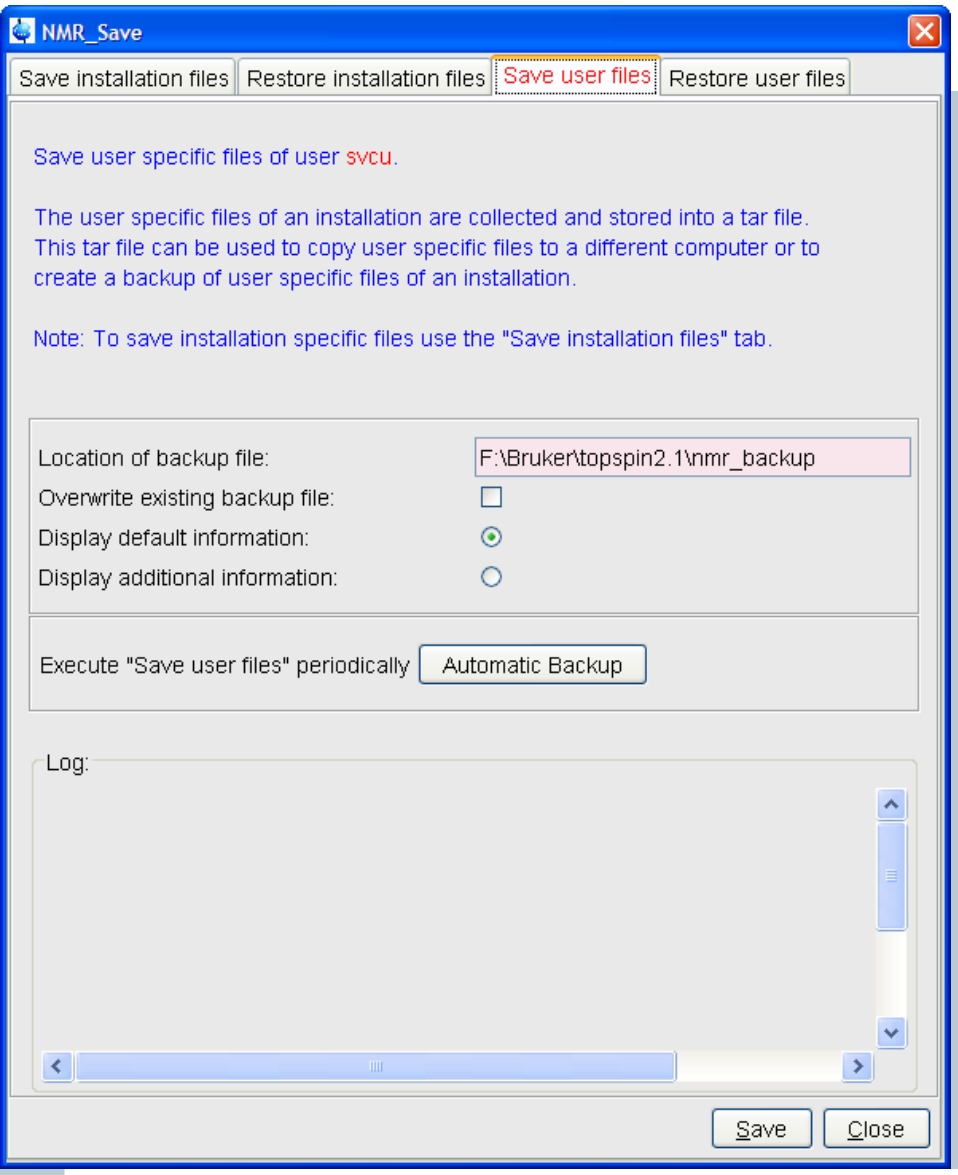


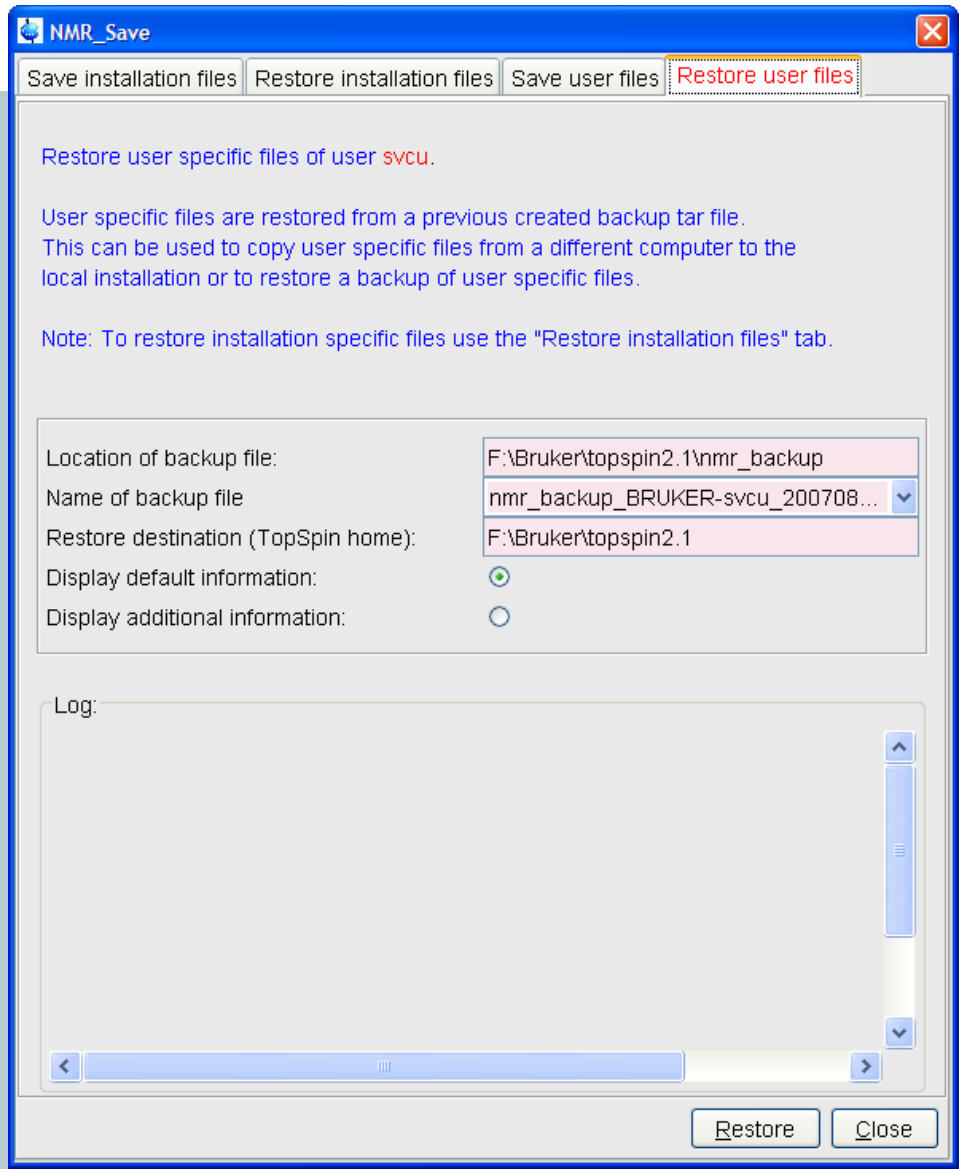
nmr_save periodically

The name of the backup files contain now date and time information, so that a periodic backup will not overwrite previous files.

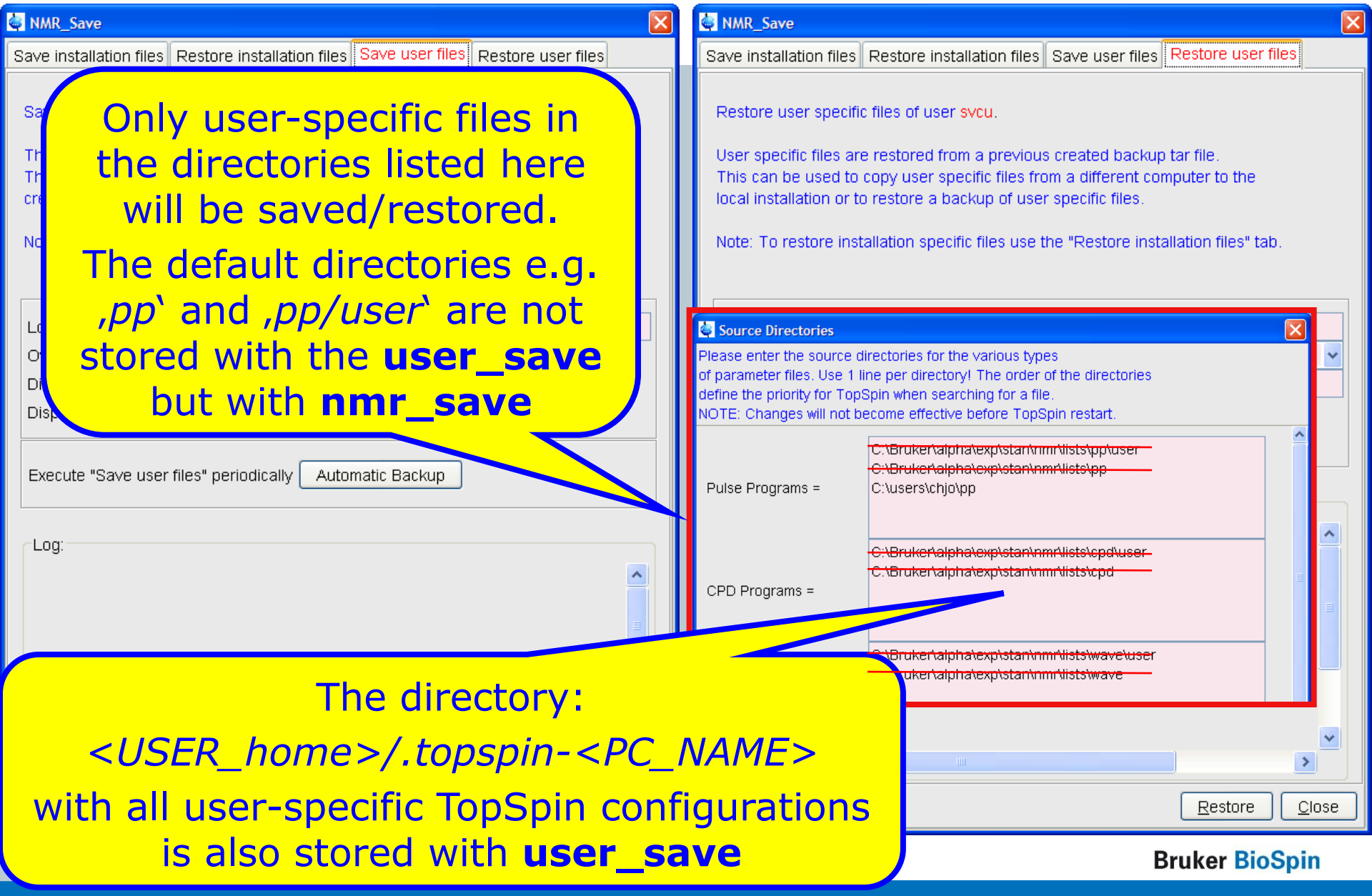


user_save/restore

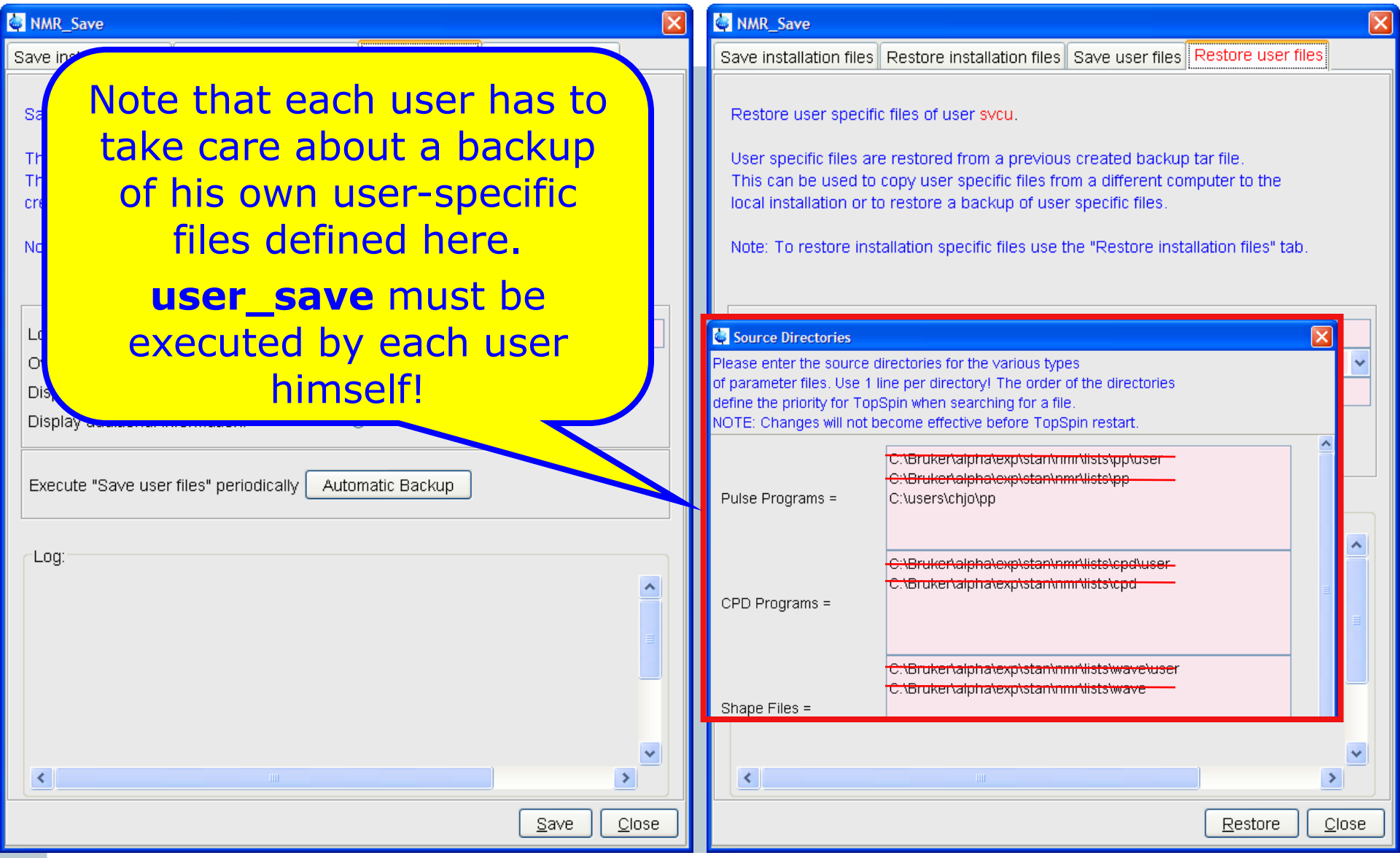




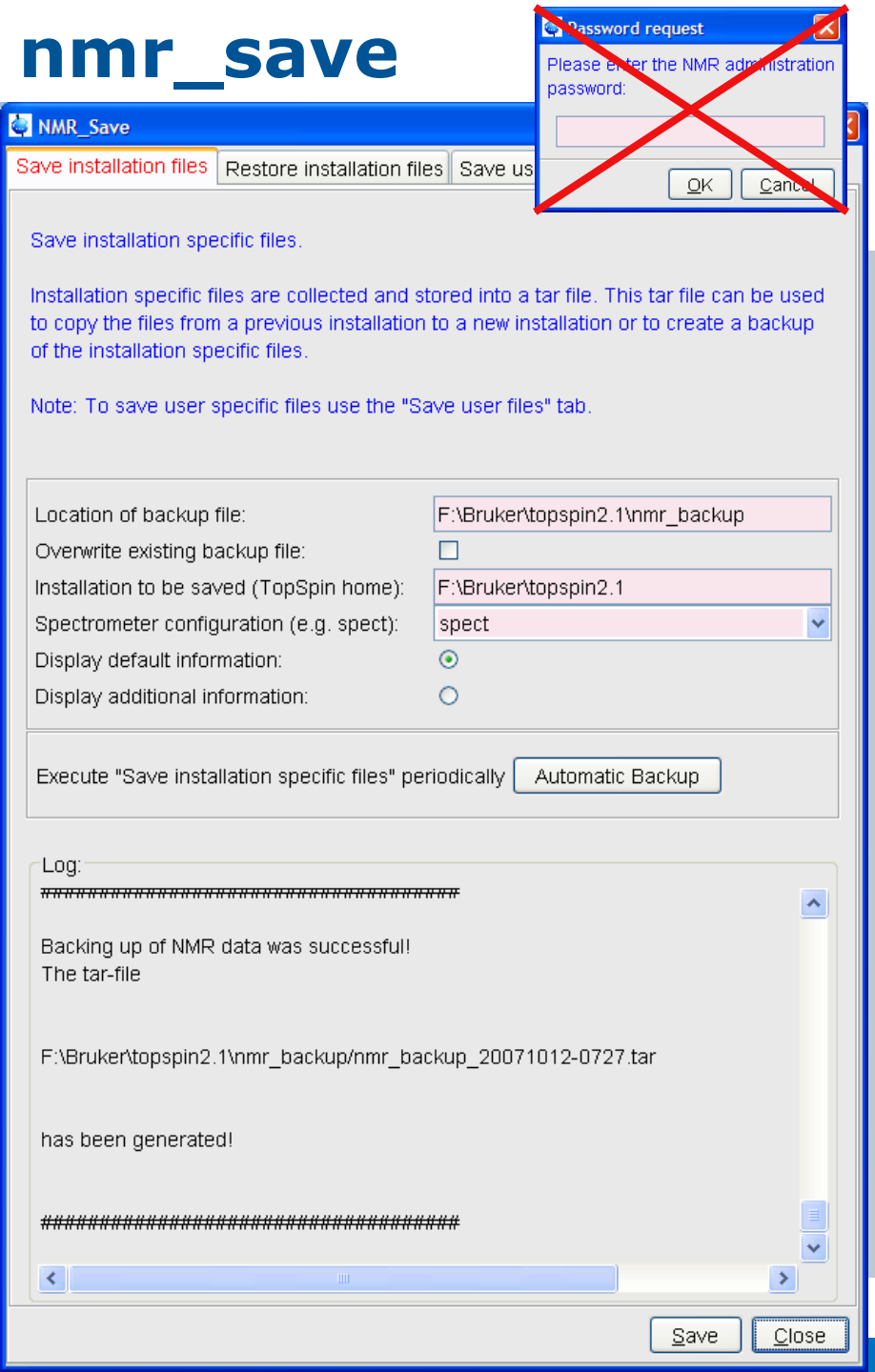
user_save/restore

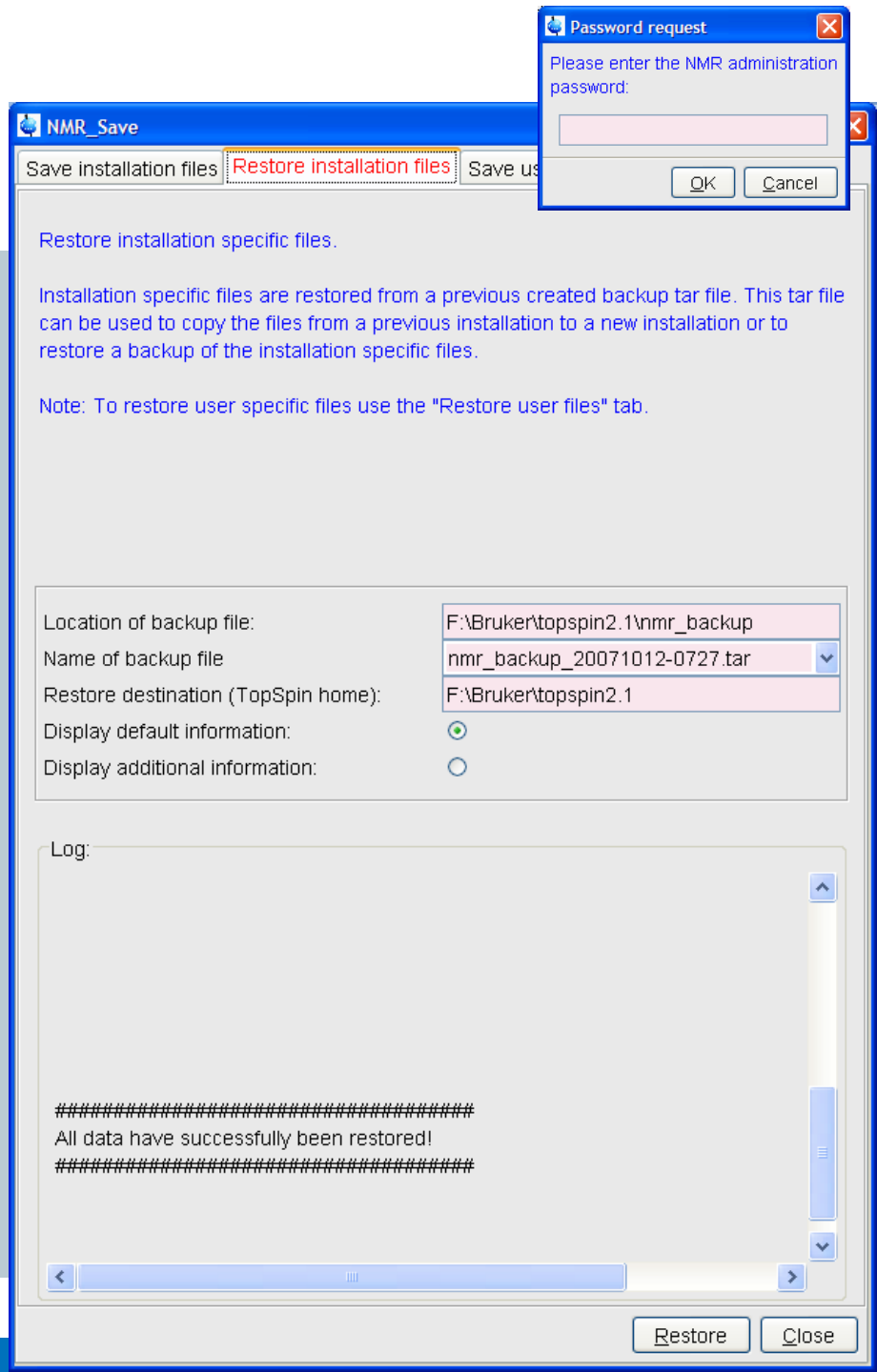


user_save/restore

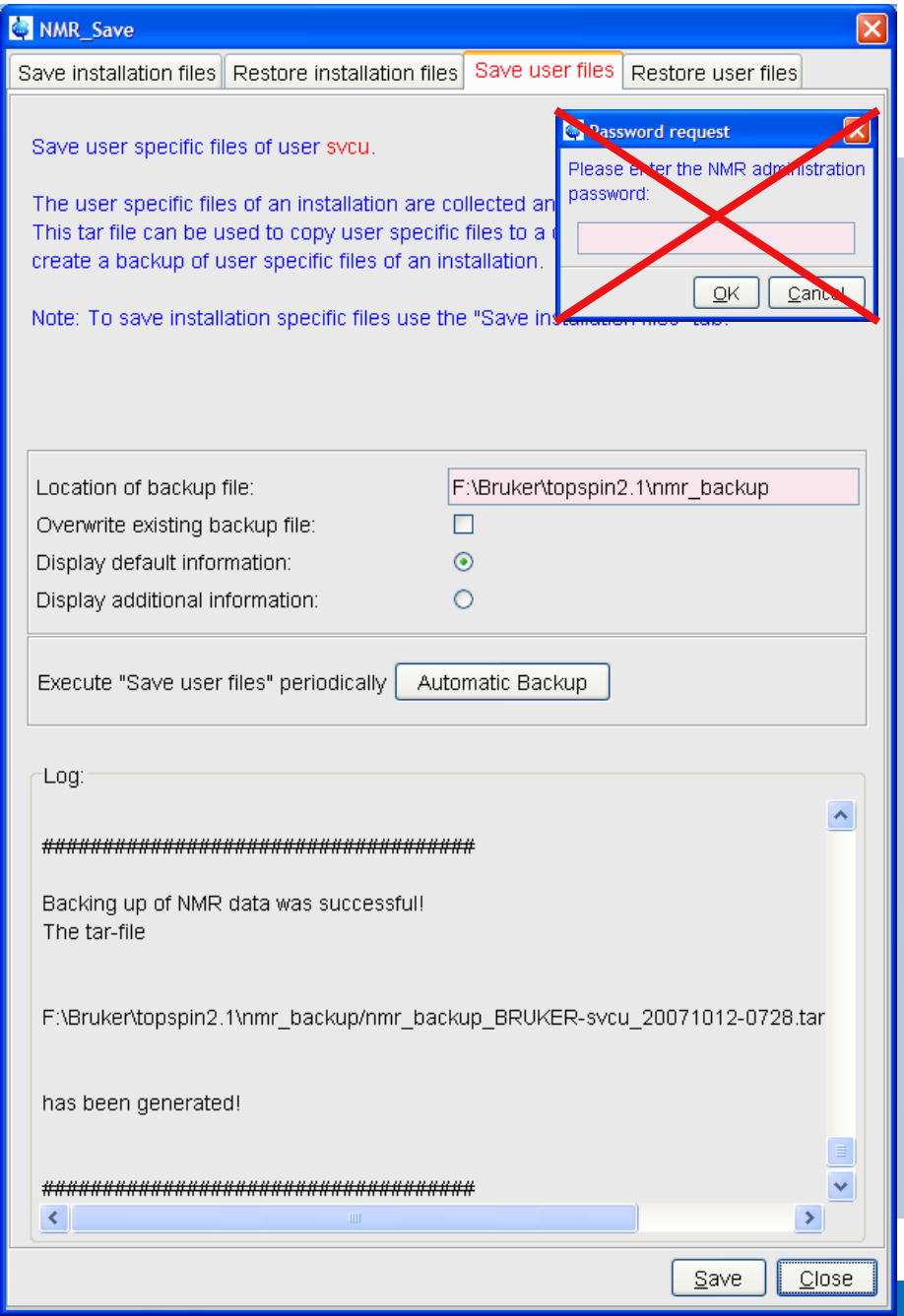


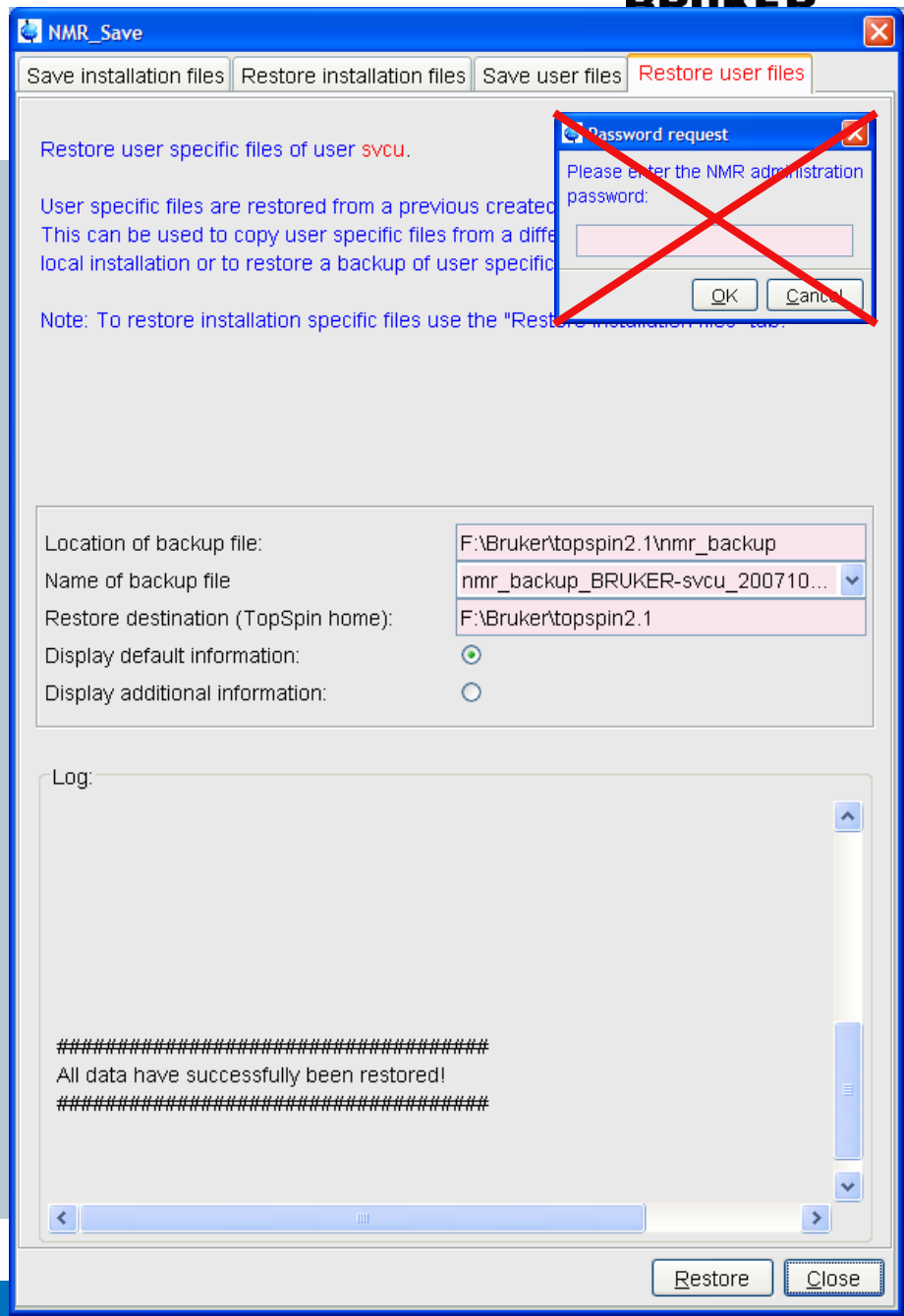
nmr_save


Password request
Please enter the NMR administration password:
OK
Cancel
NMR_Save
Save installation files
Restore installation files
Save us
Save installation specific files.
Installation specific files are collected and stored into a tar file. This tar file can be used to copy the files from a previous installation to a new installation or to create a backup of the installation specific files.
Note: To save user specific files use the "Save user files" tab.
Location of backup file:
F:\Bruker\topspin2.1\nmr_backup
Overwrite existing backup file:
Installation to be saved (TopSpin home):
F:\Bruker\topspin2.1
Spectrometer configuration (e.g. spect):
spect
Display default information:
Display additional information:
Execute "Save installation specific files" periodically
Automatic Backup
Log:
Backing up of NMR data was successful!
The tar-file
F:\Bruker\topspin2.1\nmr_backup/nmr_backup_20071012-0727.tar
has been generated!
Save
Close

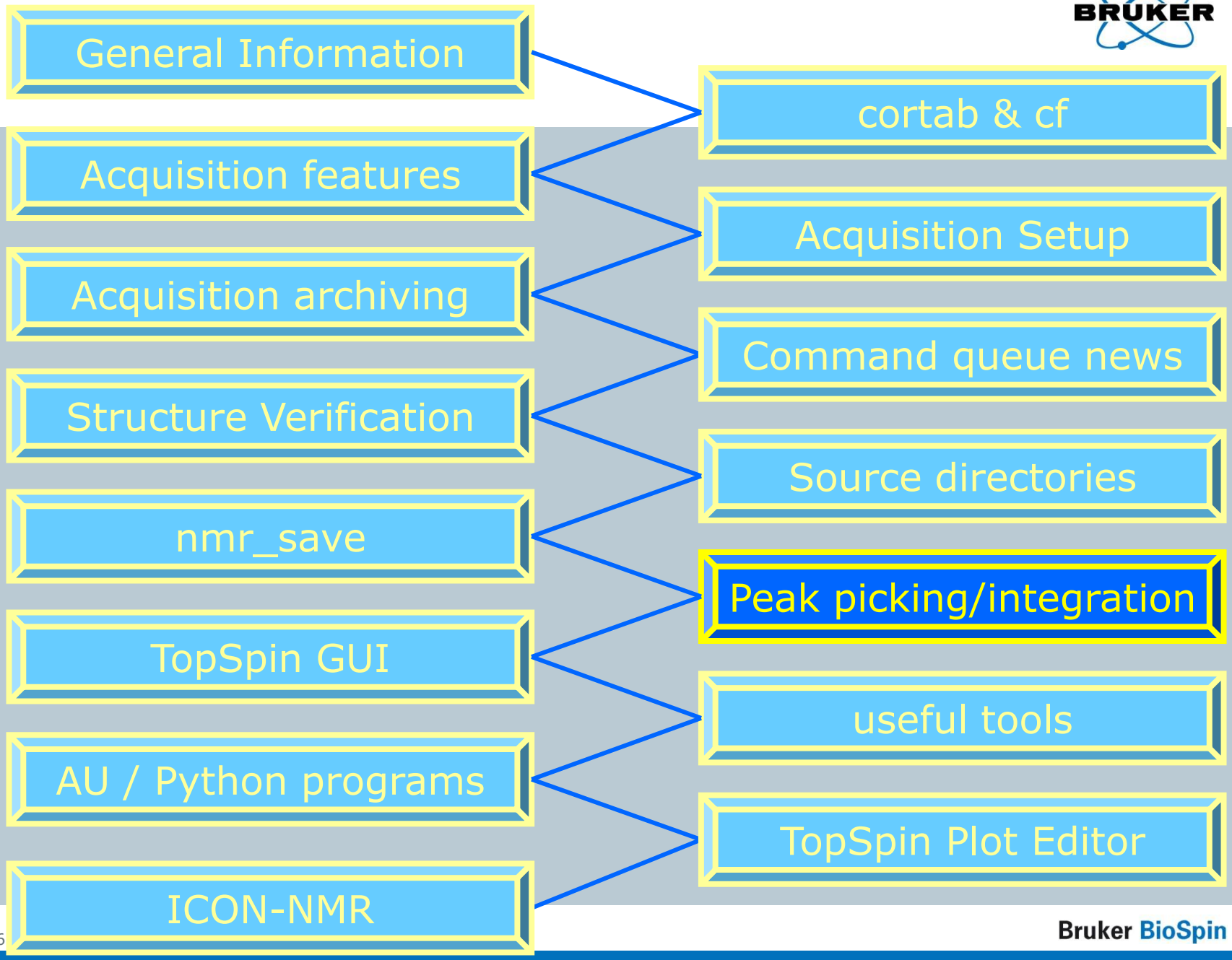

Password request
Please enter the NMR administration password:
OK
Cancel
NMR_Save
Save installation files
Restore installation files
Save us
Restore installation specific files.
Installation specific files are restored from a previous created backup tar file. This tar file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files.
Note: To restore user specific files use the "Restore user files" tab.
Location of backup file:
F:\Bruker\topspin2.1\nmr_backup
Name of backup file
nmr_backup_20071012-0727.tar
Restore destination (TopSpin home):
F:\Bruker\topspin2.1
Display default information:
Display additional information:
Log:
All data have successfully been restored!
Restore
Close

user_save


NMR_Save
Save installation files
Restore installation files
Save user files
Restore user files
Save user specific files of user svcu.
The user specific files of an installation are collected an
This tar file can be used to copy user specific files to a
create a backup of user specific files of an installation.
Note: To save installation specific files use the "Save
Password request
Please enter the NMR administration password:
OK
Cancel
Location of backup file:
F:\Bruker\topspin2.1\nmr_backup
Overwrite existing backup file:
Display default information:
Display additional information:
Execute "Save user files" periodically
Automatic Backup
Log:
Backing up of NMR data was successful!
The tar-file
F:\Bruker\topspin2.1\nmr_backup/nmr_backup_BRUKER-svcu_20071012-0728.tar
has been generated!
Save
Close


NMR_Save
Save installation files
Restore installation files
Save user files
Restore user files
Restore user specific files of user svcu.
User specific files are restored from a previous created
This can be used to copy user specific files from a diffe
local installation or to restore a backup of user specific
Note: To restore installation specific files use the "Rest
Password request
Please enter the NMR administration password:
OK
Cancel
Location of backup file:
F:\Bruker\topspin2.1\nmr_backup
Name of backup file
nmr_backup_BRUKER-svcu_200710...
Restore destination (TopSpin home):
F:\Bruker\topspin2.1
Display default information:
Display additional information:
Log:
All data have successfully been restored!
Restore
Close

Content


General Information
Acquisition features
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Structure Verification
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ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

Peak picking 1D

TopSpin < 2.1

TopSpin stores peaks as text file

TopSpin 2.1

TopSpin stores peaks as XML file

next page

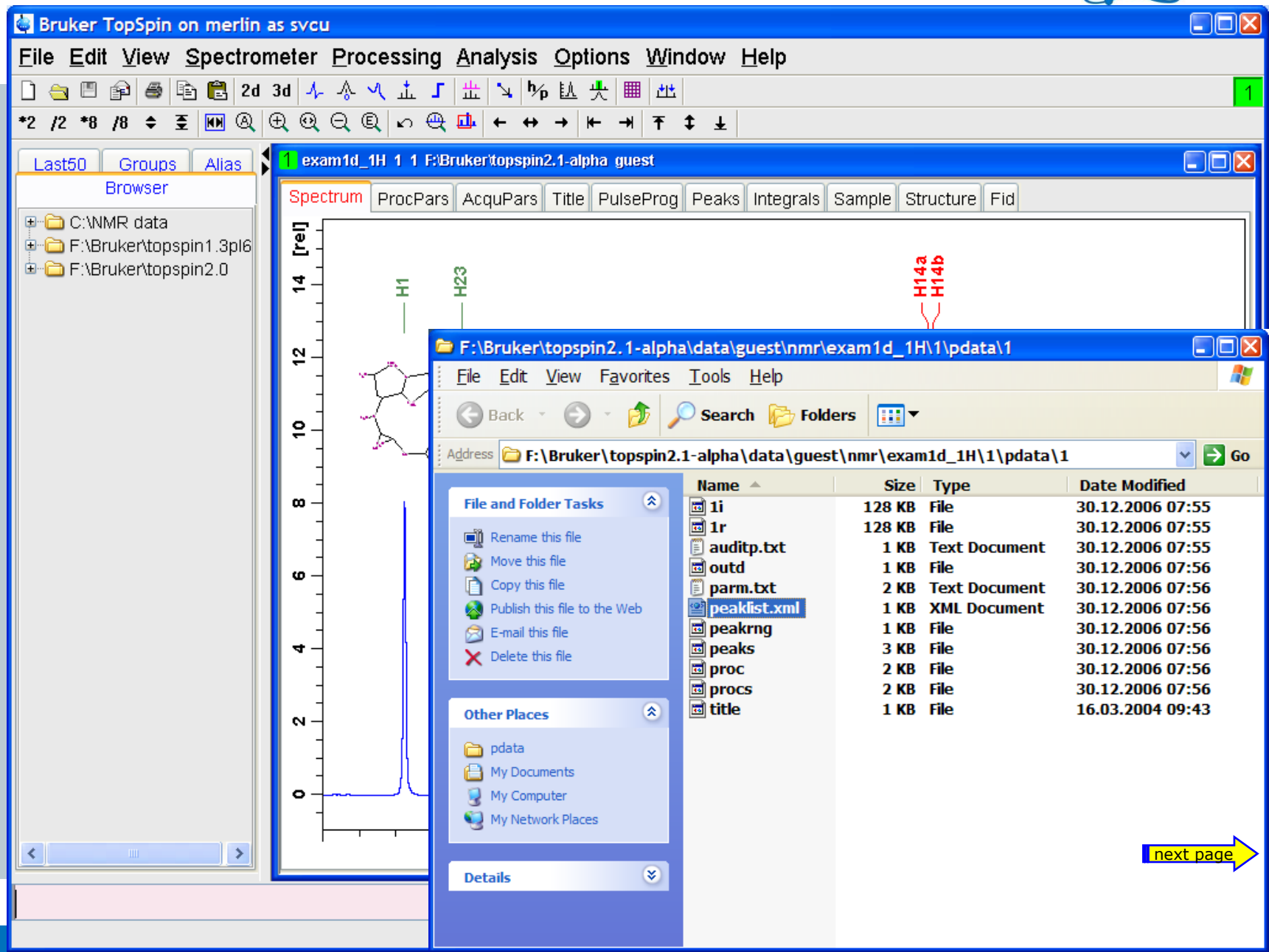
Peak picking 1D

TopSpin 2.1 stores peaks in the XML file peaklist.xml

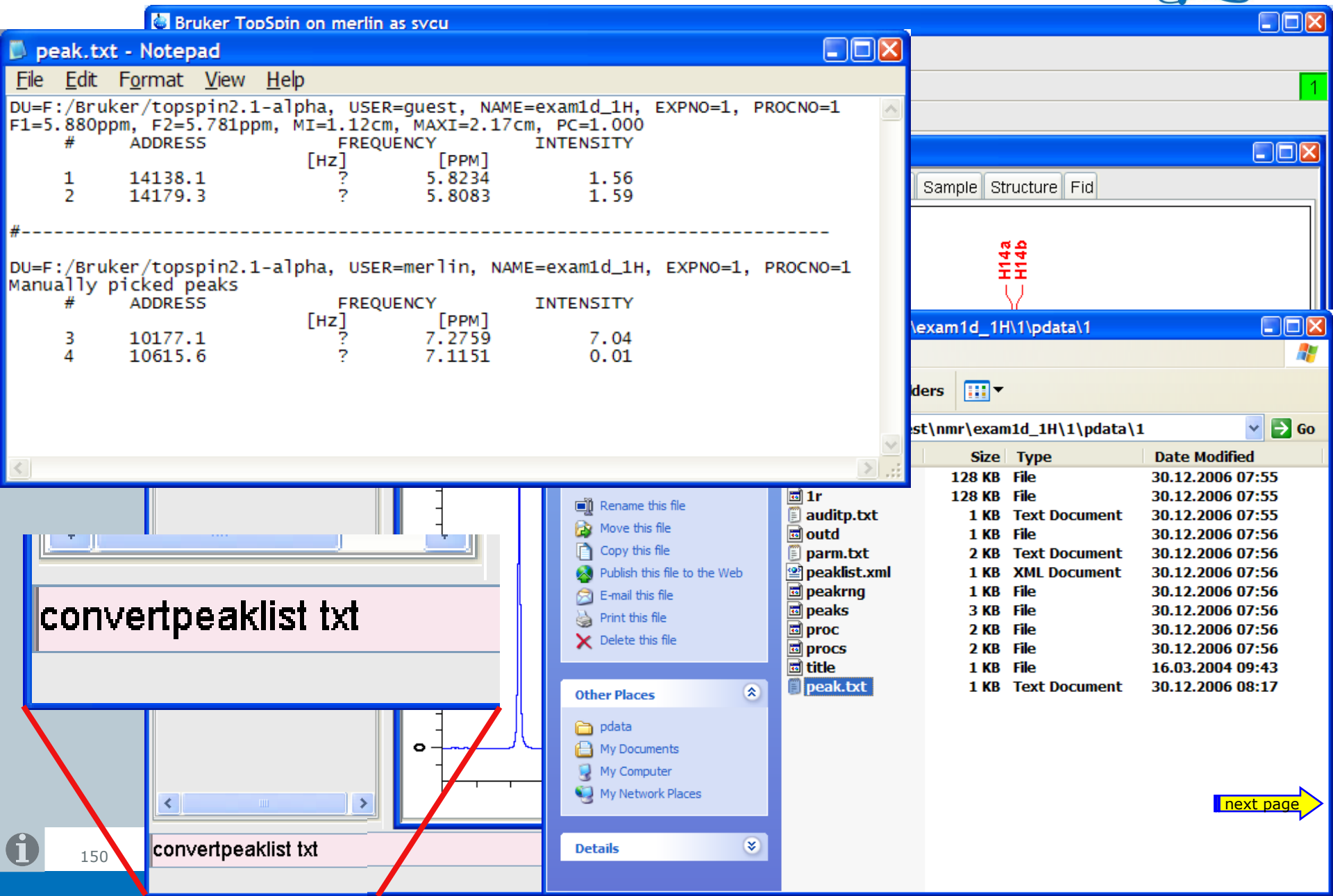
- New features are possible (see following)
- but if AU/third party programs are used to parse the old file (peak.txt) a conversion has to be done
- for this the command **convertpeaklist txt** is implemented

next page

Peak picking 1D



Peak picking 1D



Peak picking 1D

Bruker TopSpin on merlin as svcu

peak.txt - Notepad

File Edit Format View Help

```
DU=F:/Bruker/topspin2.1-alpha, USER=guest, NAME=exam1d_1H, EXPNO=1,
F1=5.880ppm, F2=5.781ppm, MI=1.12cm  MAXI=2.17cm, PC=1.000
     #      ADDRESS              FREQUENCY              INTENSITY
                              [Hz]          [PPM]
     1      14138.1                ?         5.8234          1.56
     2      14179.3                ?         5.8083          1.59

#------------------------------------------------------------------

DU=F:/Bruker/topspin2.1-alpha, USER=merlin, NAME=exam1d_1H, EXPNO=1,
Manually picked peaks
     #      ADDRESS              FREQUENCY              INTENSITY
                              [Hz]          [PPM]
     3      10177.1                ?         7.2759          7.04
     4      10615.6                ?         7.1151          0.01
```

Note:
Because peak.txt
is created manually
it could be outdated!

⟹

Whenever TopSpin
modify the peaklist
it will move the
textfile peak.txt
to peak.txt.bak

Rename this file
Move this file
Copy this file
Publish this file to the Web
E-mail this file
Print this file
Delete this file

Other Places
pdata
My Documents
My Computer
My Network Places

Details

next page

Peak picking 1D

What about datasets/peak lists created with TopSpin < 2.1?

When these datasets are opened with TopSpin 2.1 the file peak.txt is automatically converted in:
peaklist.xml
and the original file peak.txt is renamed into peak.txt.bak

next page

Peak picking 1D

Please note that if you have user-specific AU programs with peak picking AND if the peak file is used for any further procedures you have to modify your setup.

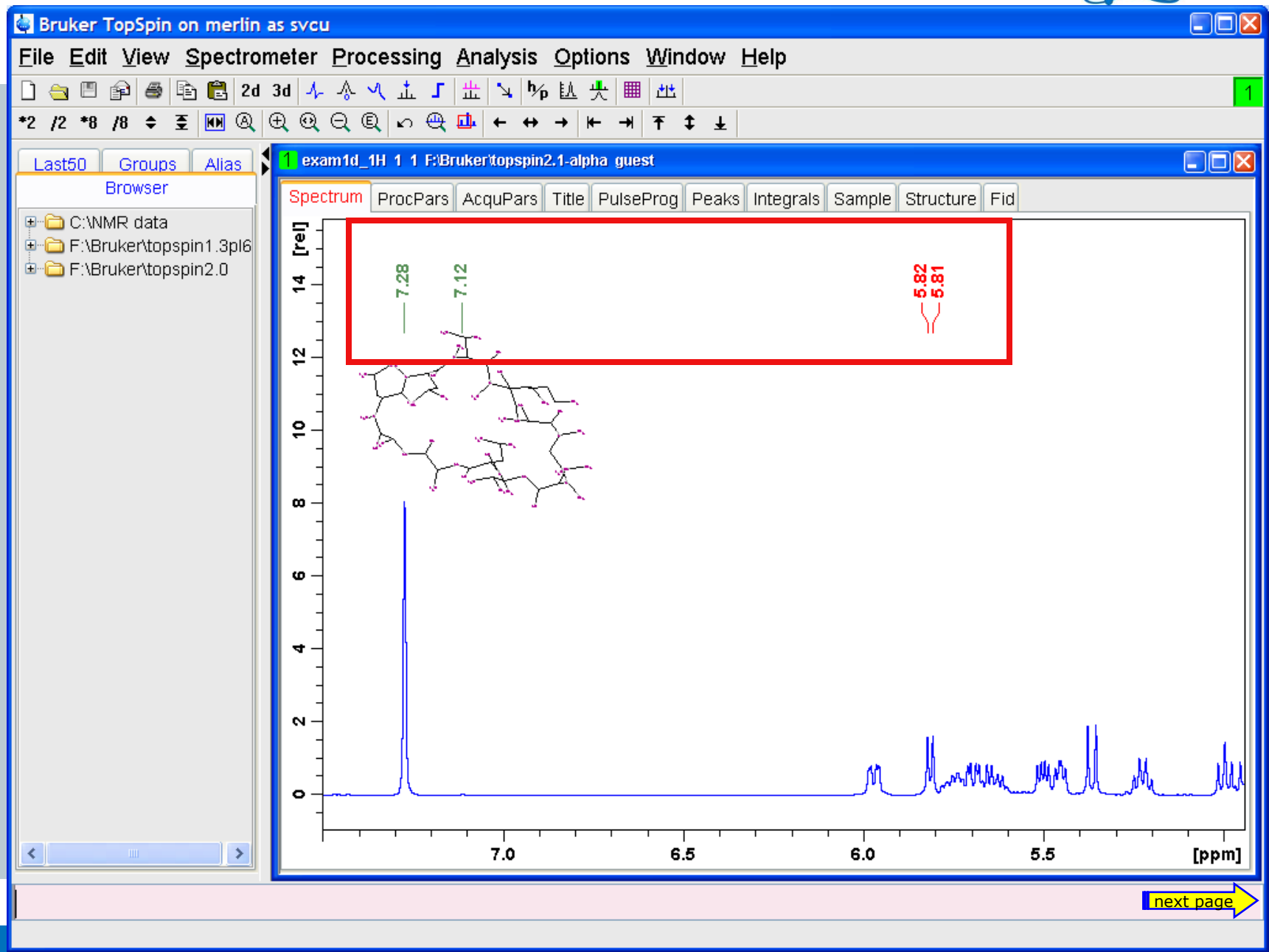
For more details check the
Release Letter of TopSpin 2.1.

next page

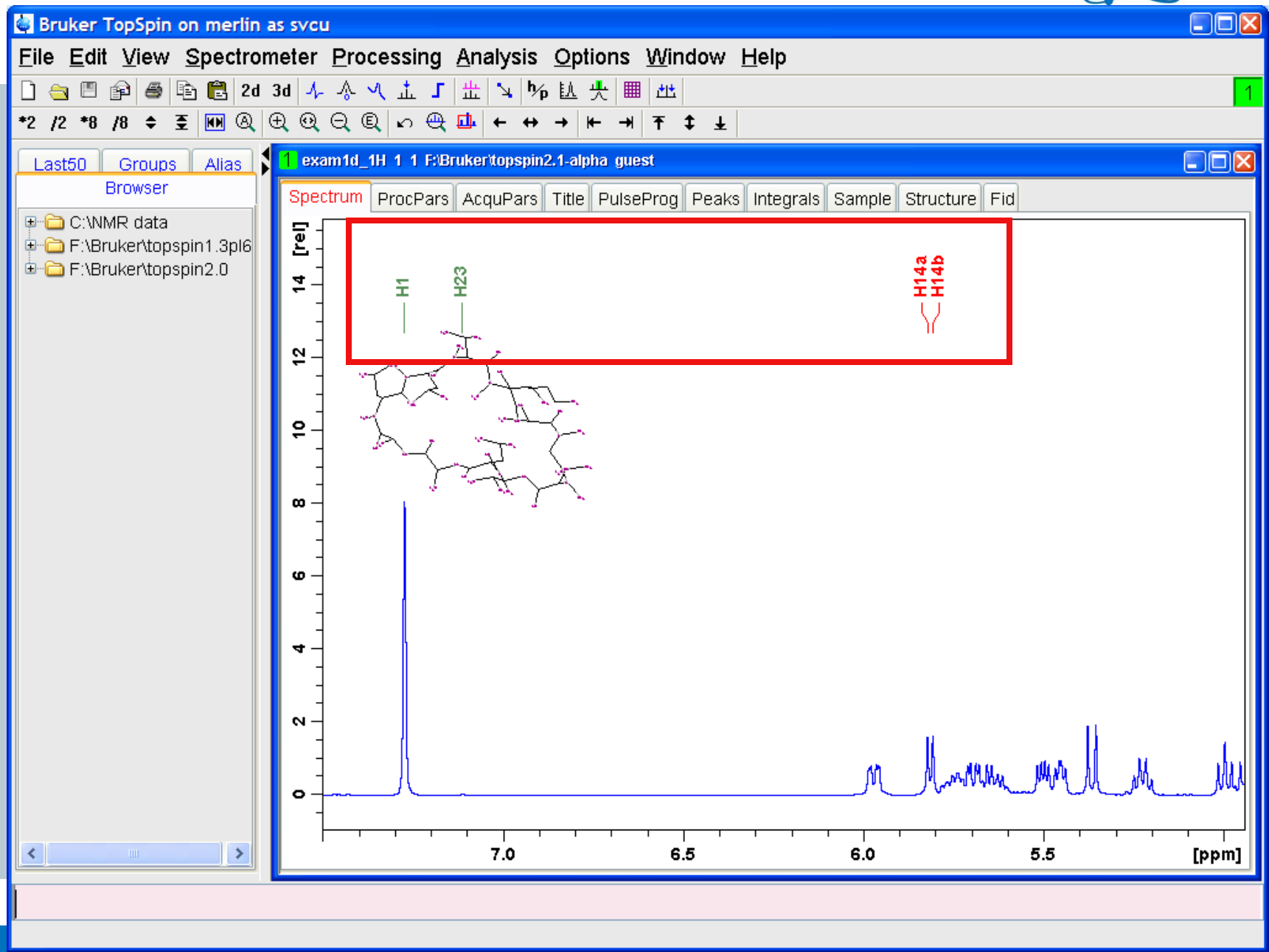
Peak picking 1D

Because of the new format peaklist created with TopSpin 2.1 can not be displayed with XWIN-NMR / TopSpin < 2.1.

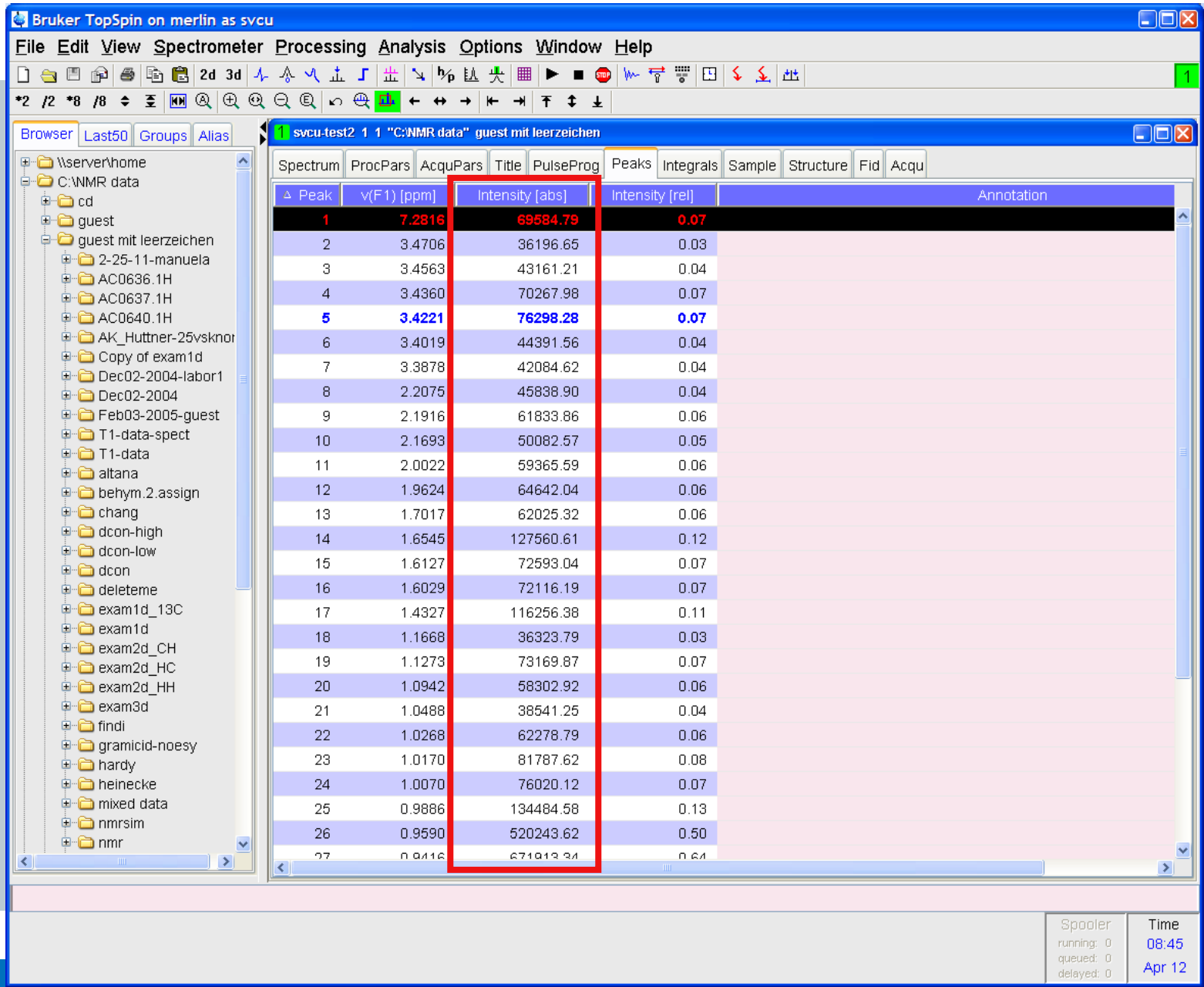
Peak picking 1D



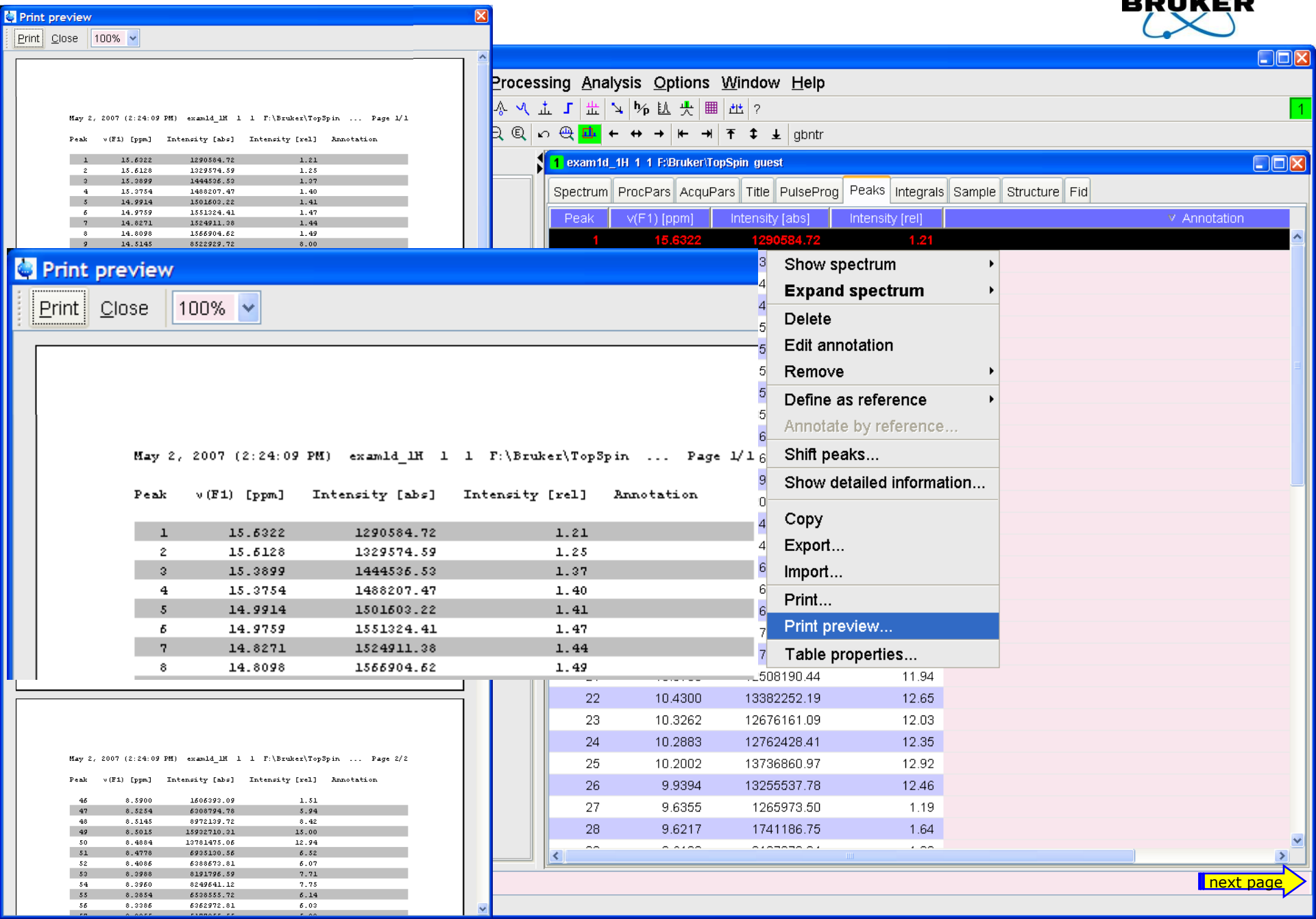
Peak picking 1D: annotations



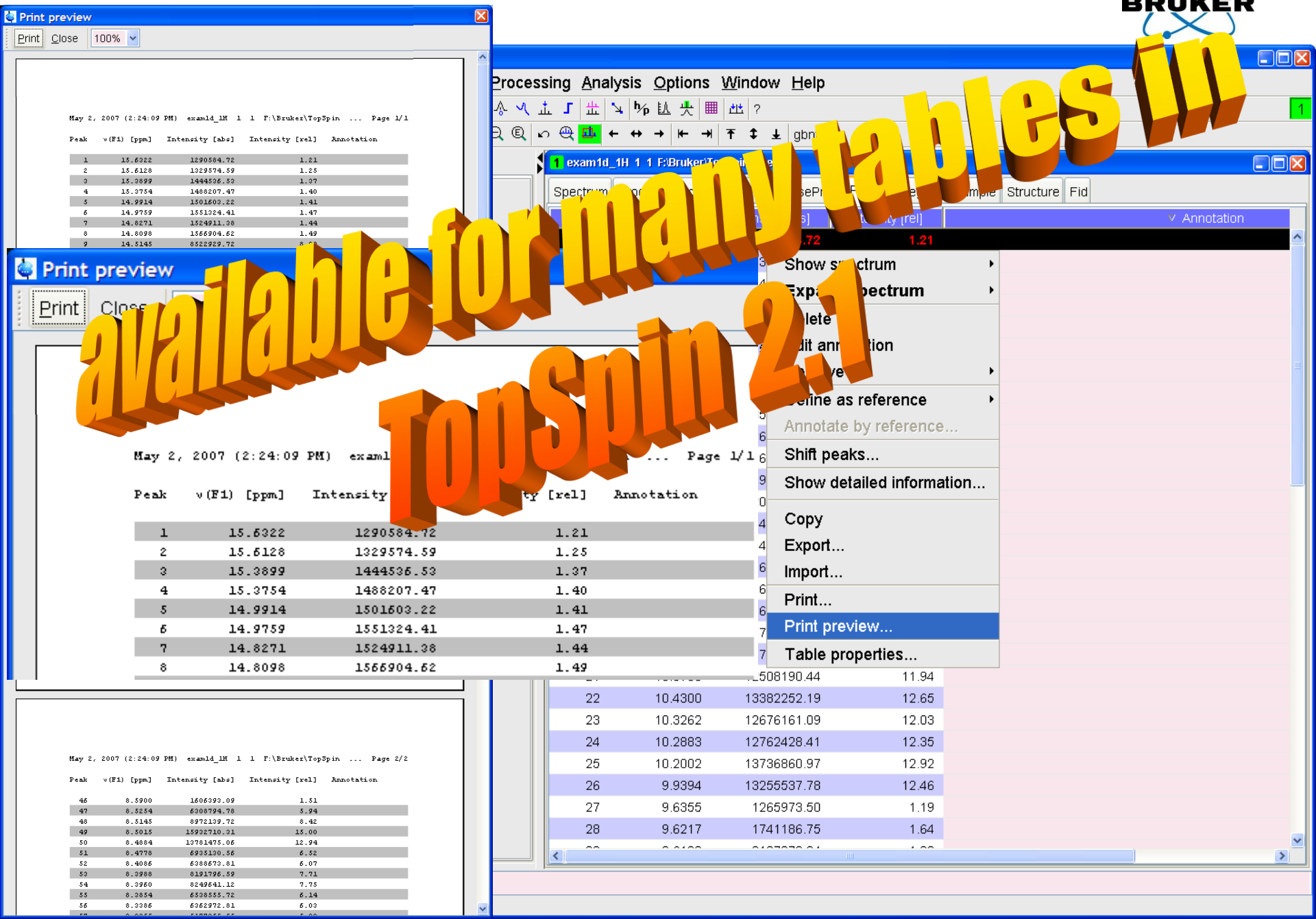
Peak picking 1D: absolute values



Peak picking 1D: print preview available

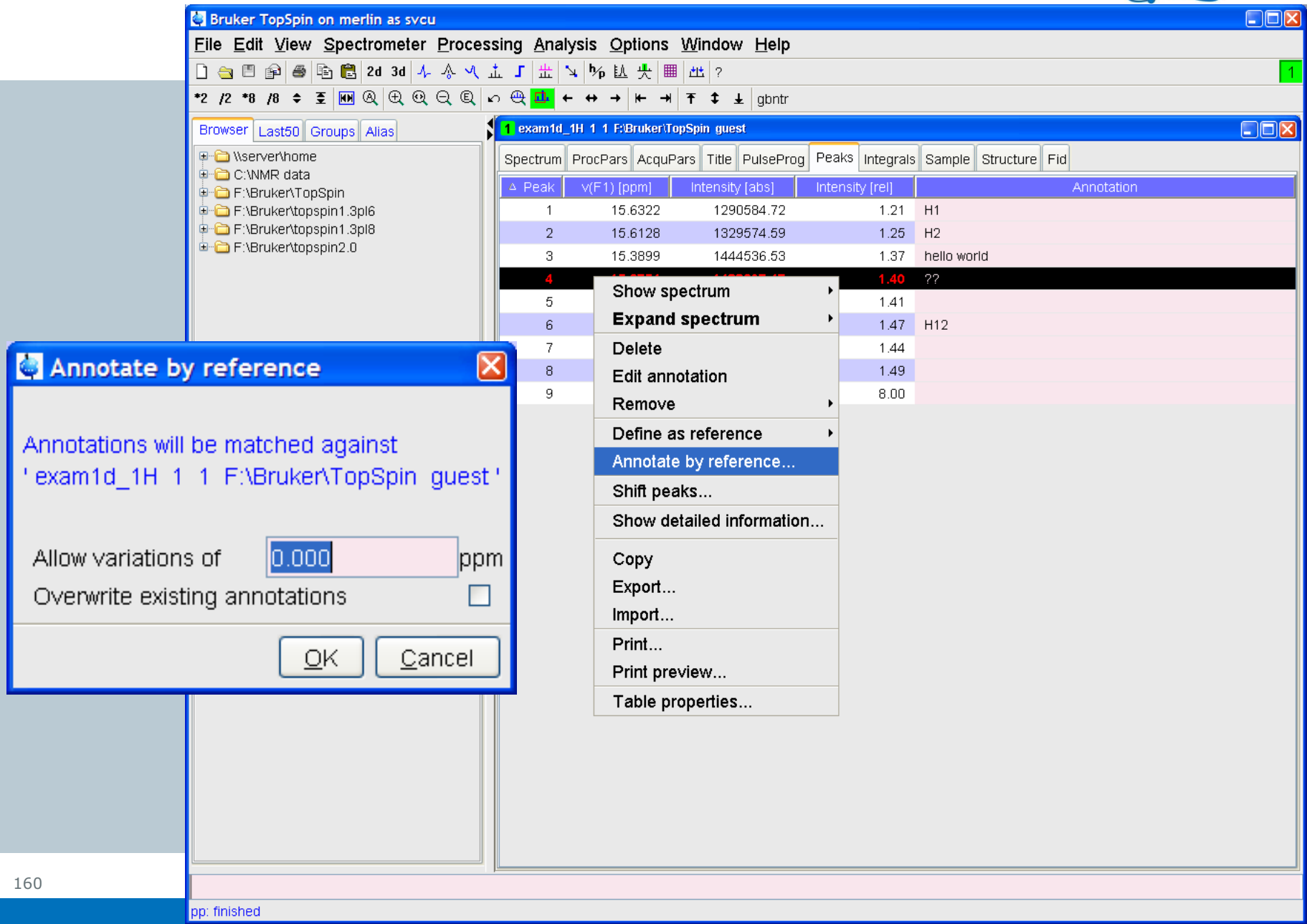


Peak picking 1D: print preview available

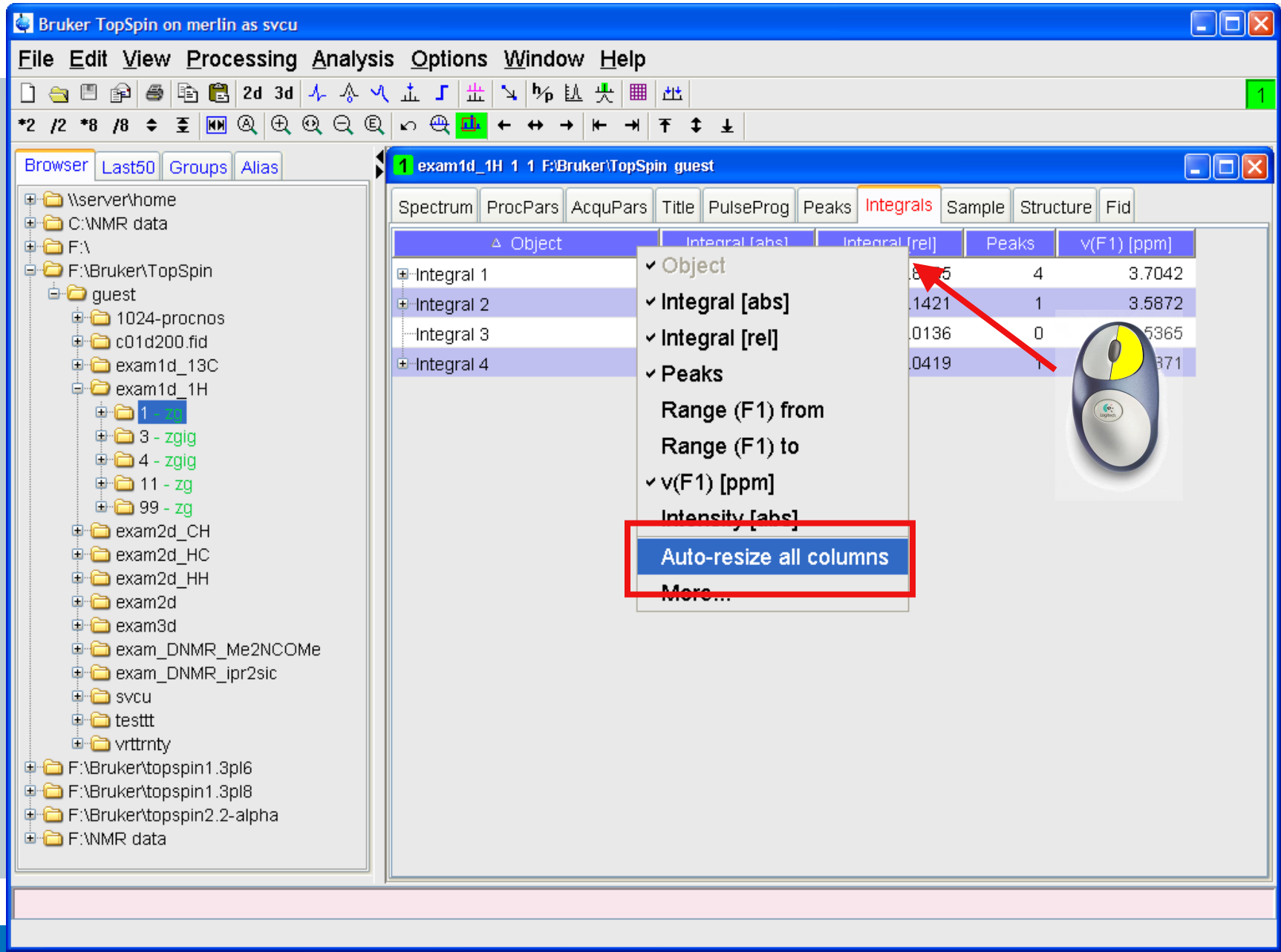


available for many tables in TopSpin 2.1

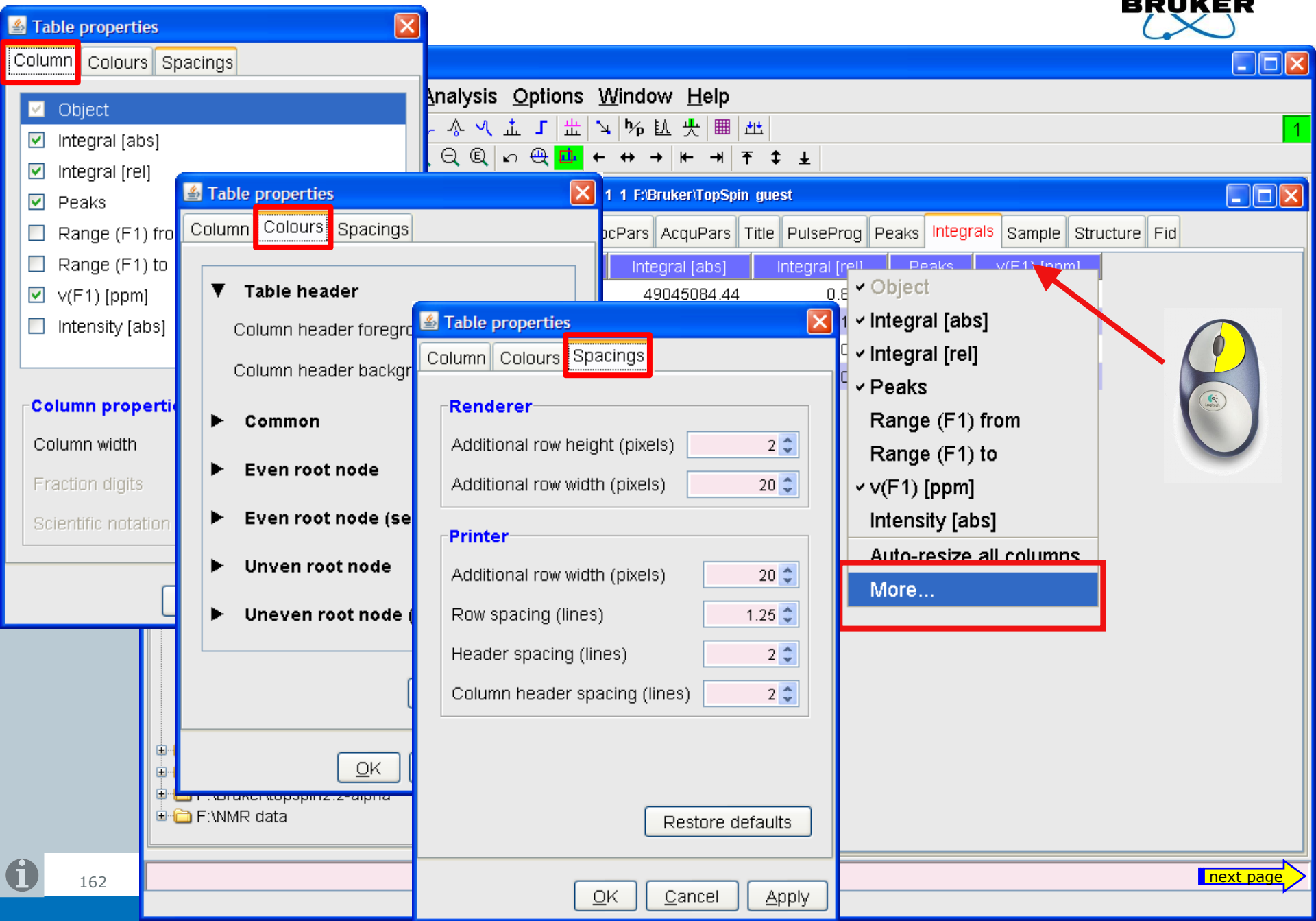
Peak picking 1D: transfer annotations



Auto-resize all columns

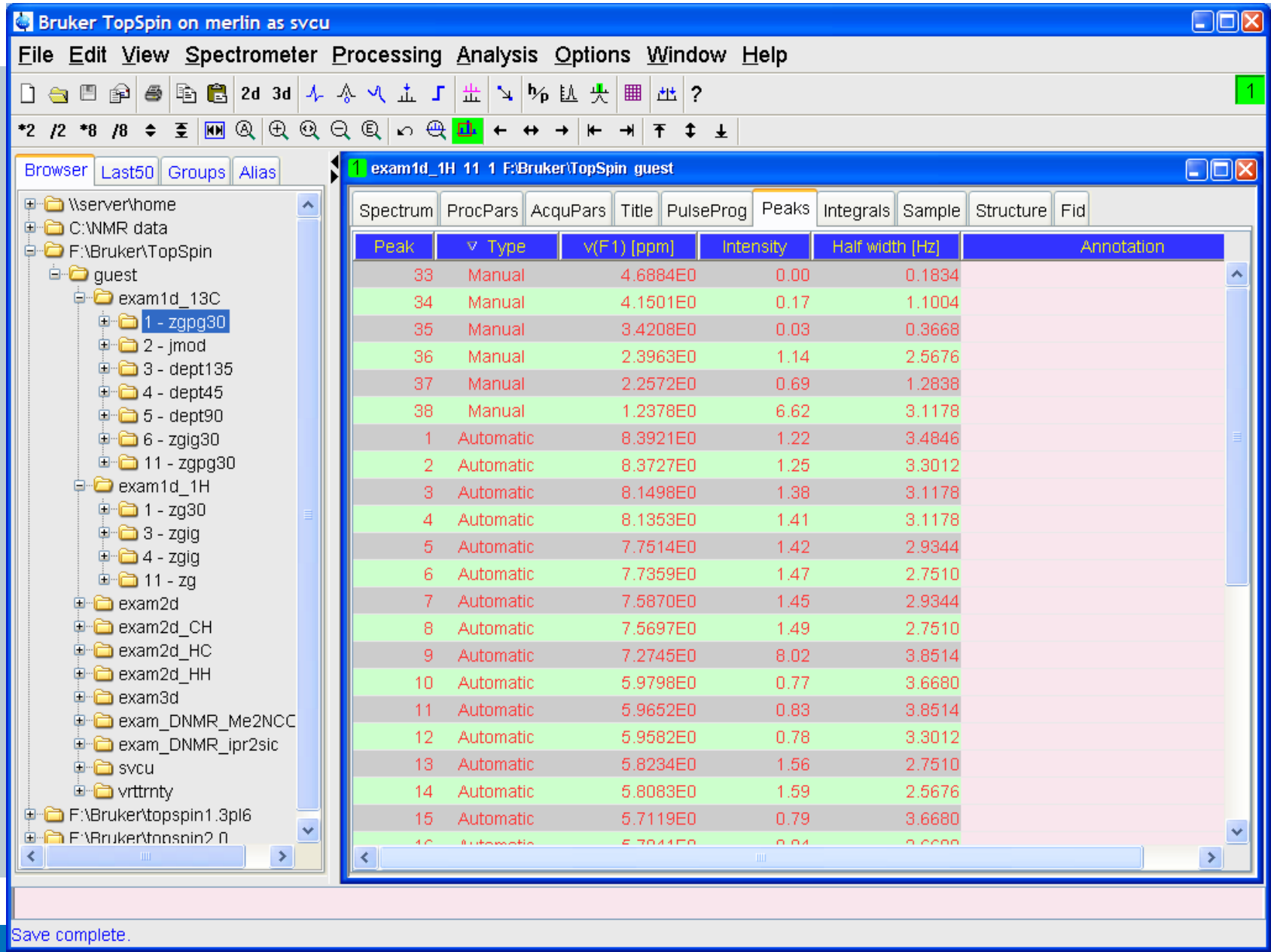


More table properties

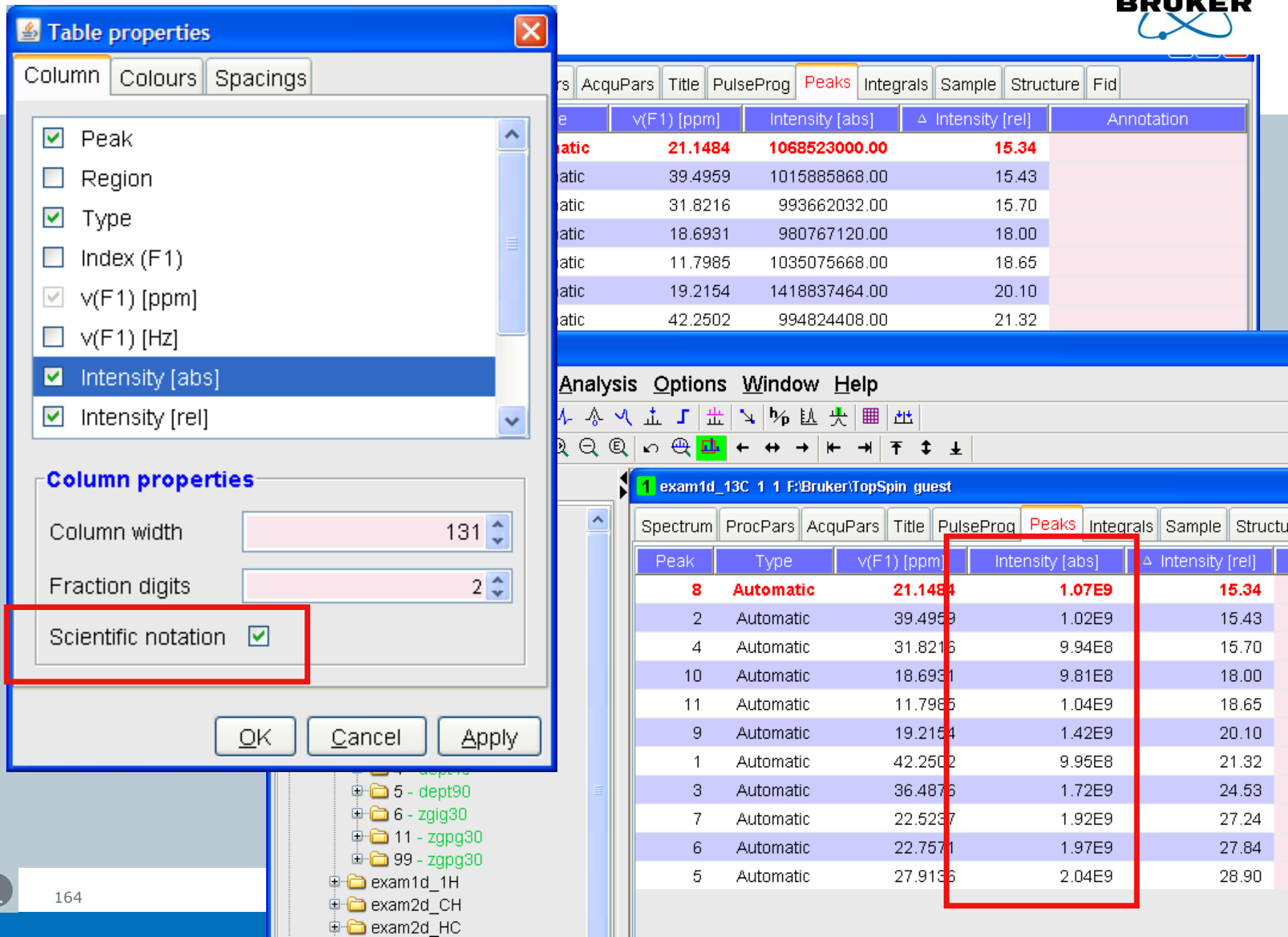


next page

An example for different table colours

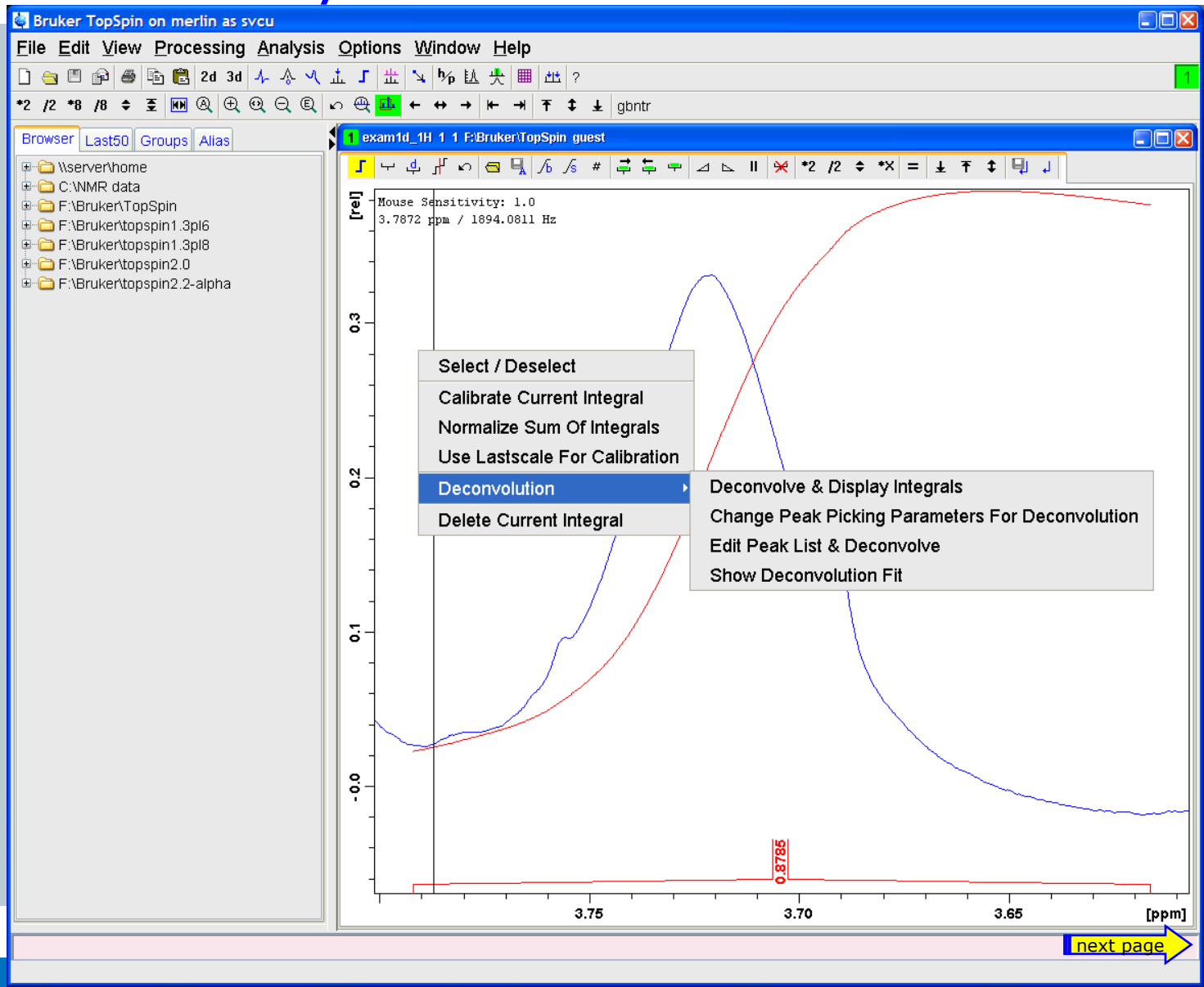


Scientific notation



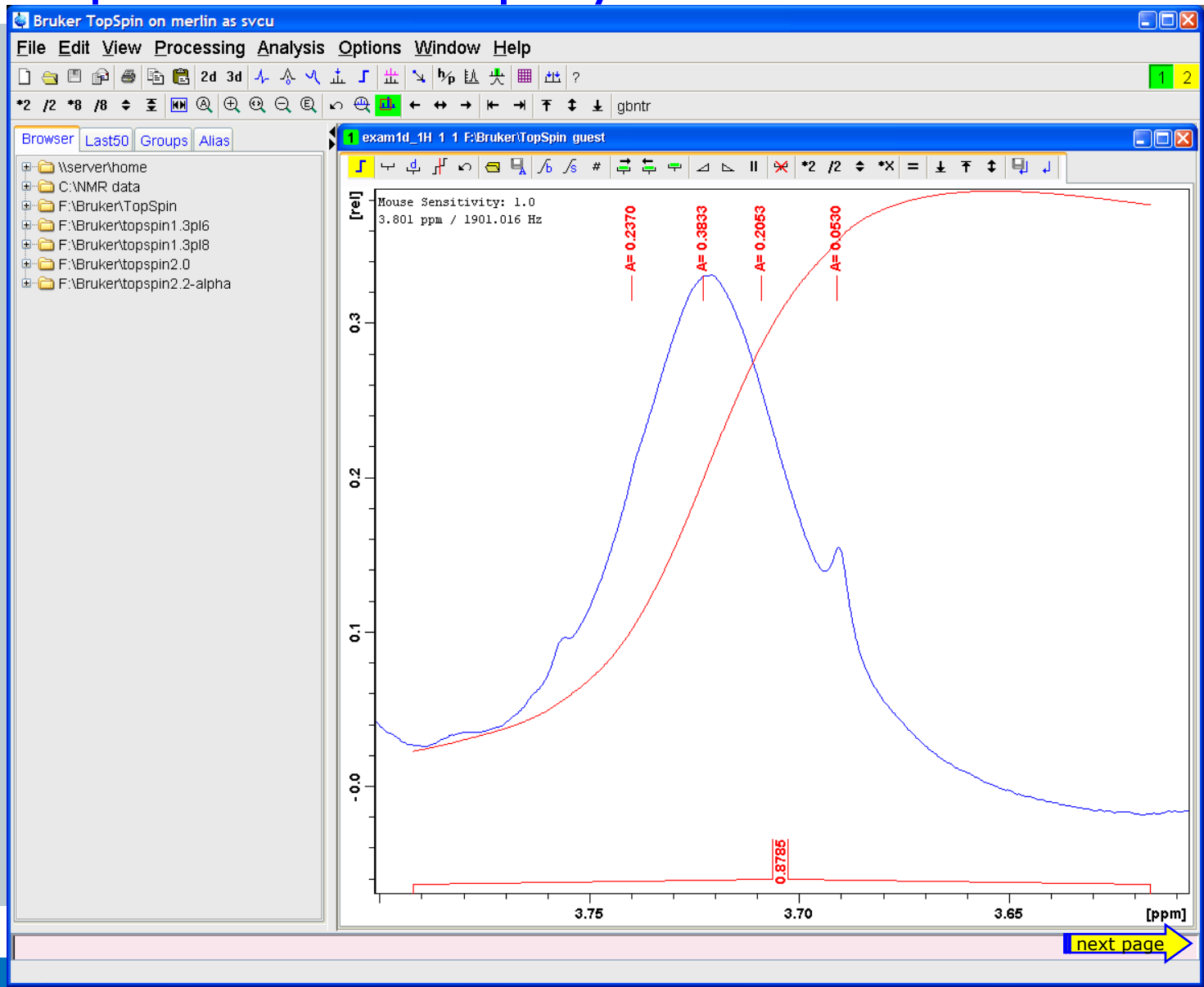
Integration of peak shoulders

Integration offers easy access to deconvolution



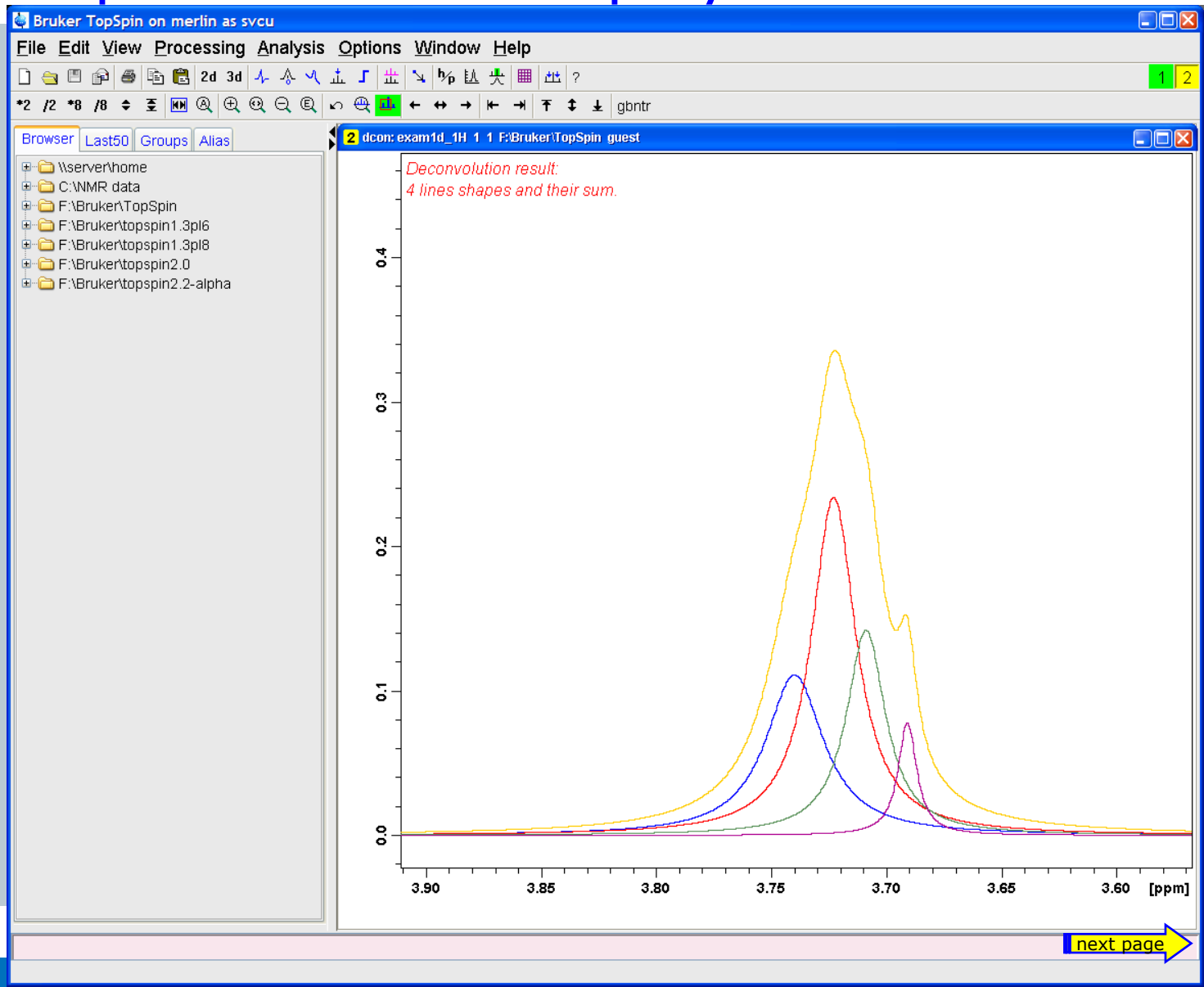
Integration of peak shoulders

Deconvoluted peaks are displayed



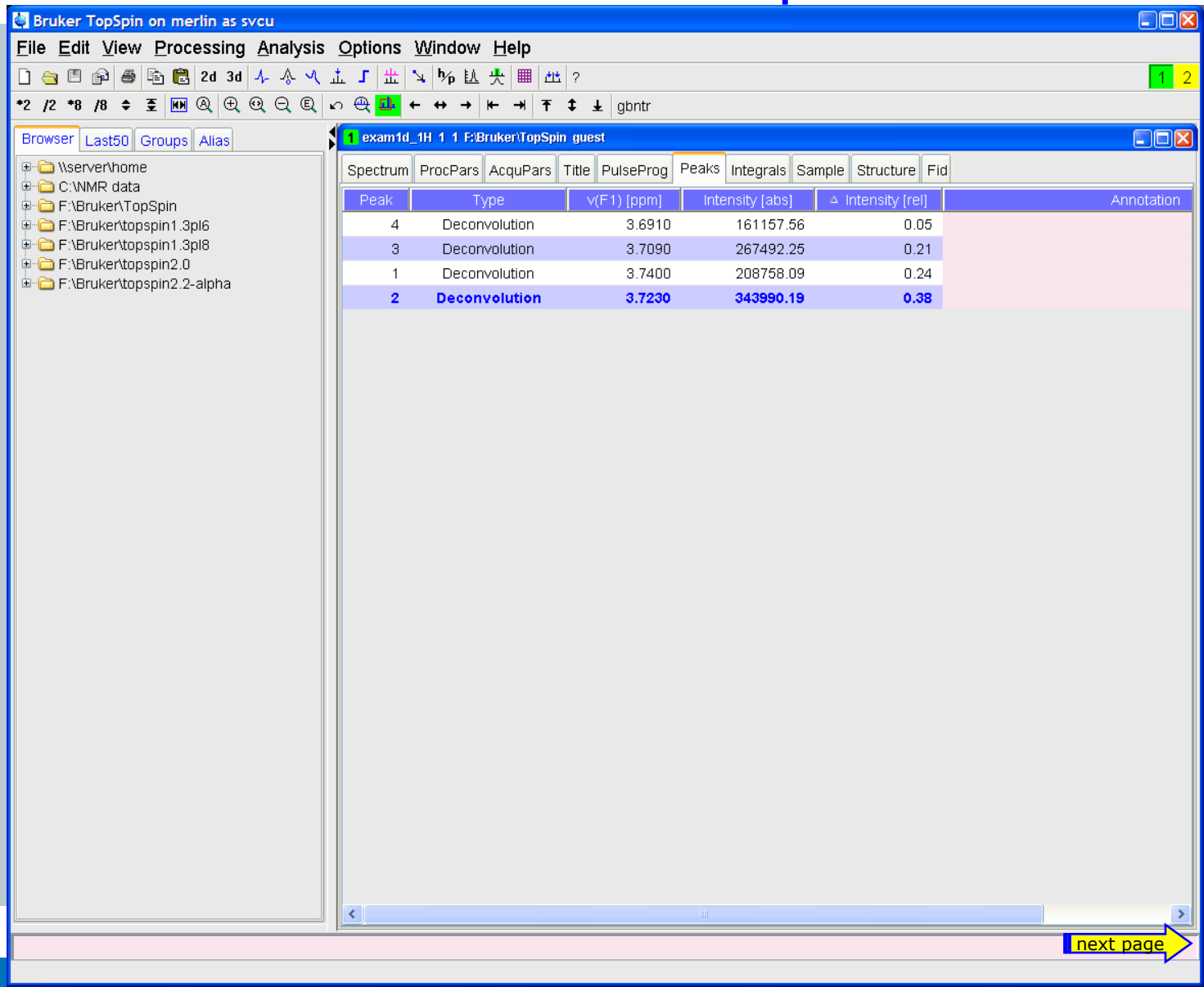
Integration of peak shoulders

Shapes of the peaks can be displayed



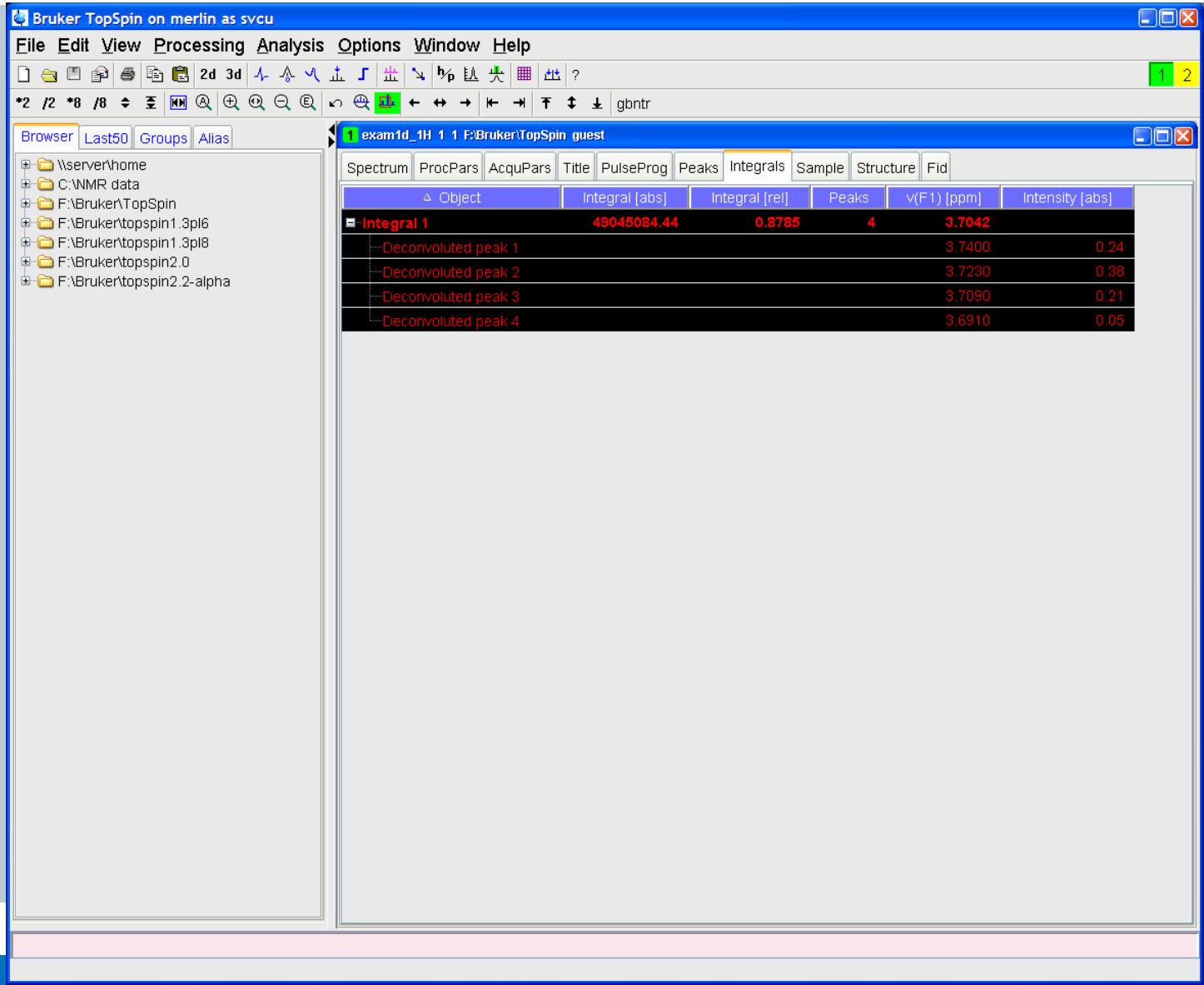
Integration of peak shoulders

Peak list contains also deconvoluted peaks

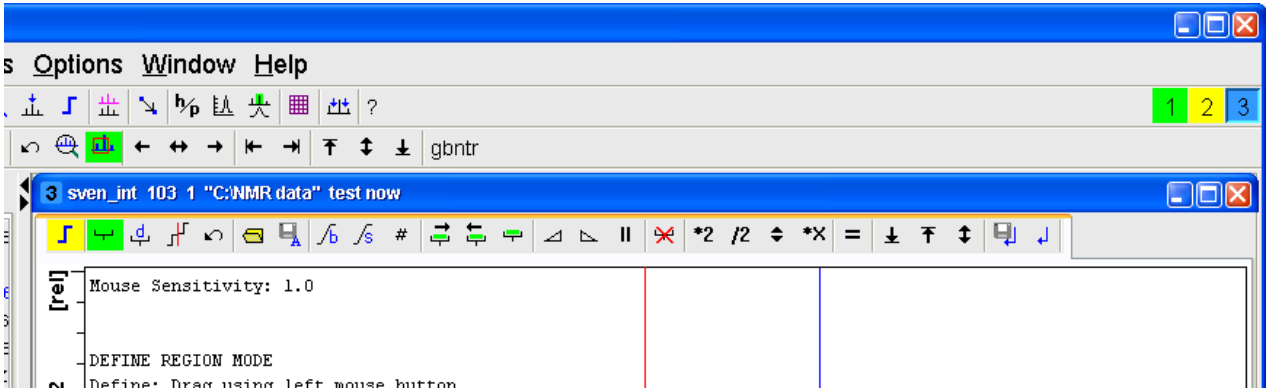


Integration of peak shoulders

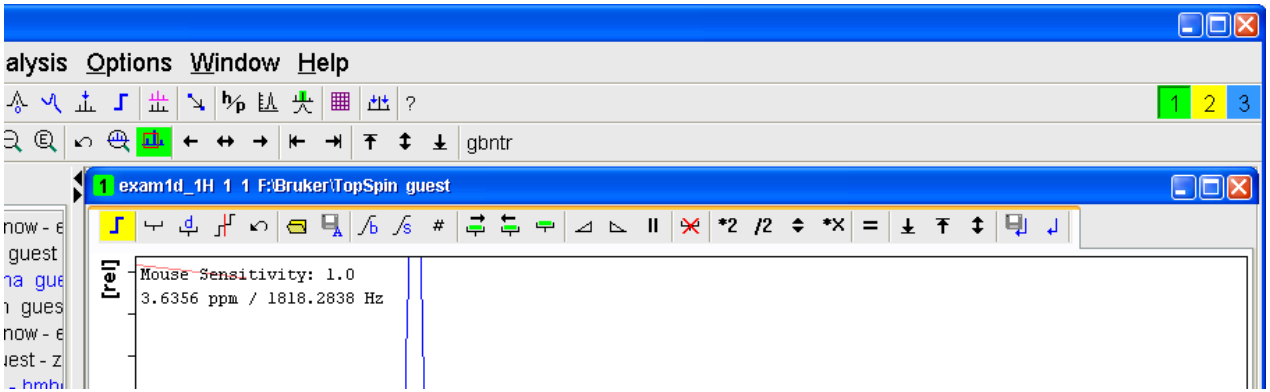
Integration list contains also intensities of decon. peaks



Behaviour of integration submenu



No integrals exist ➔ creating integrals is enabled when entering



integrals exist ➔ creating integrals is disabled when entering

nD peak lists

nD peak lists can be displayed in TopSpin.

Automatic peak picking 2D/3D

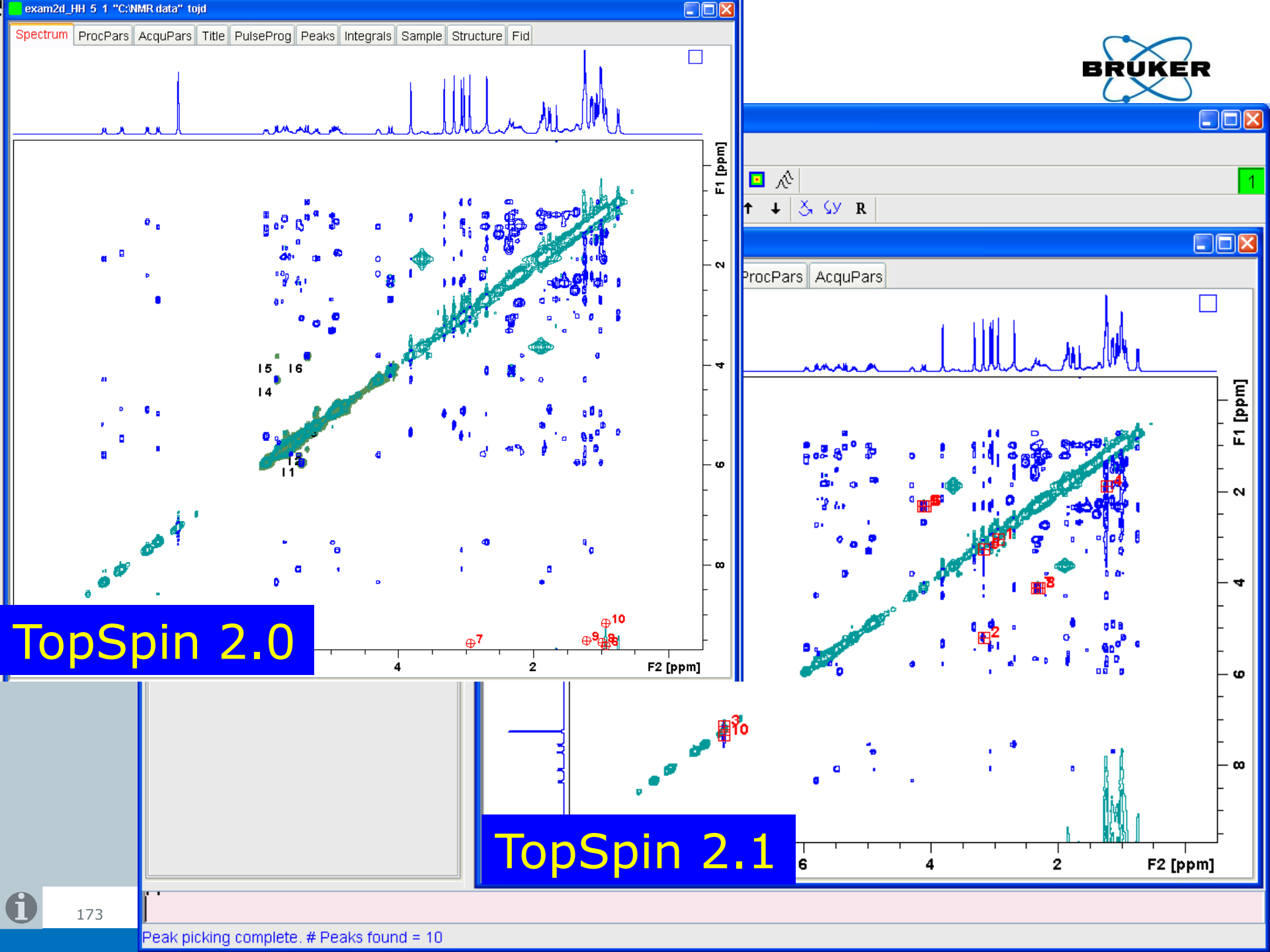
TopSpin < 2.1

TopSpin picks as many peaks
as defined in **PPMPNUM**

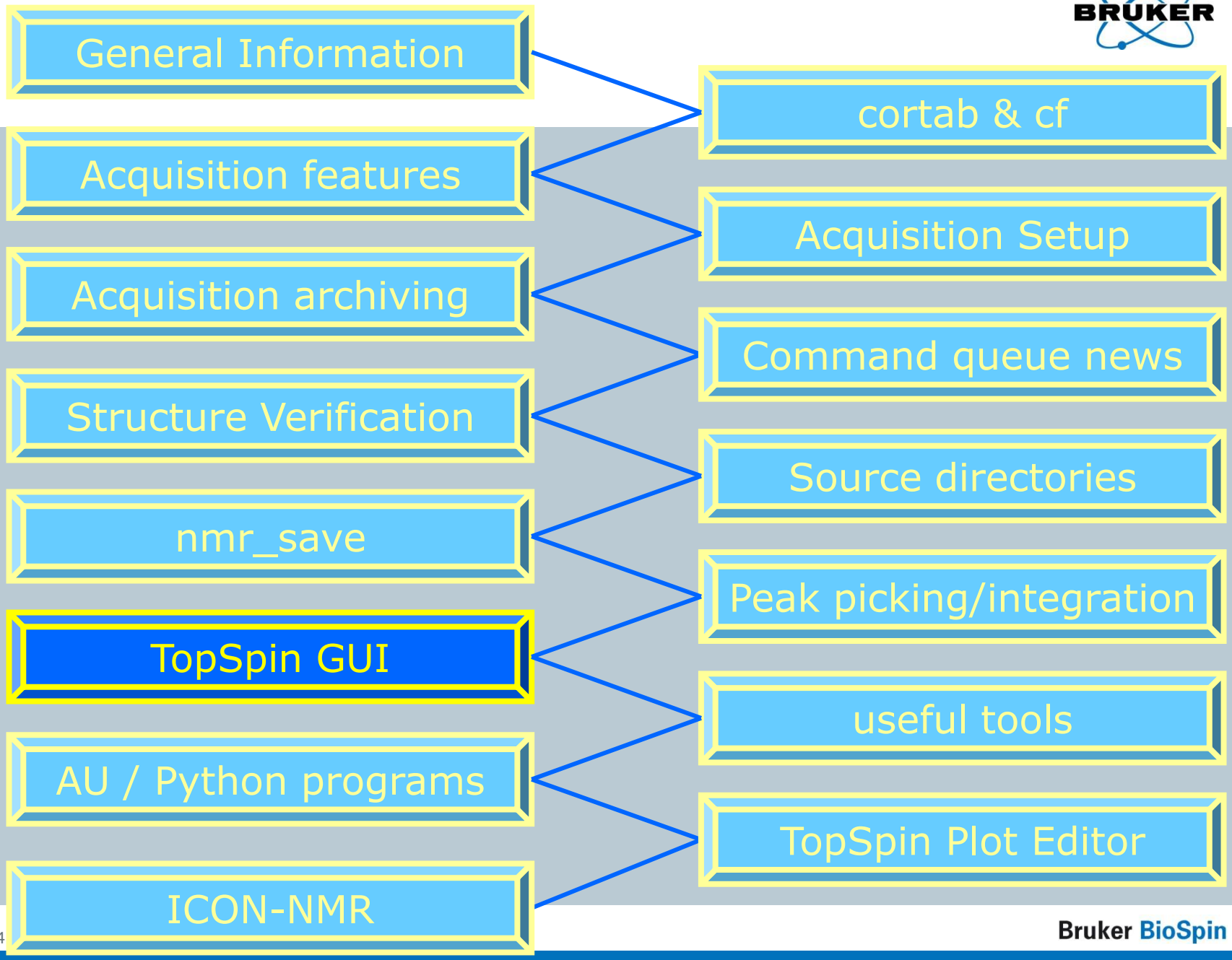
TopSpin 2.1

TopSpin picks all peaks
- the most intensive ones will be displayed
- as many as defined in **PPMPNUM**

next page

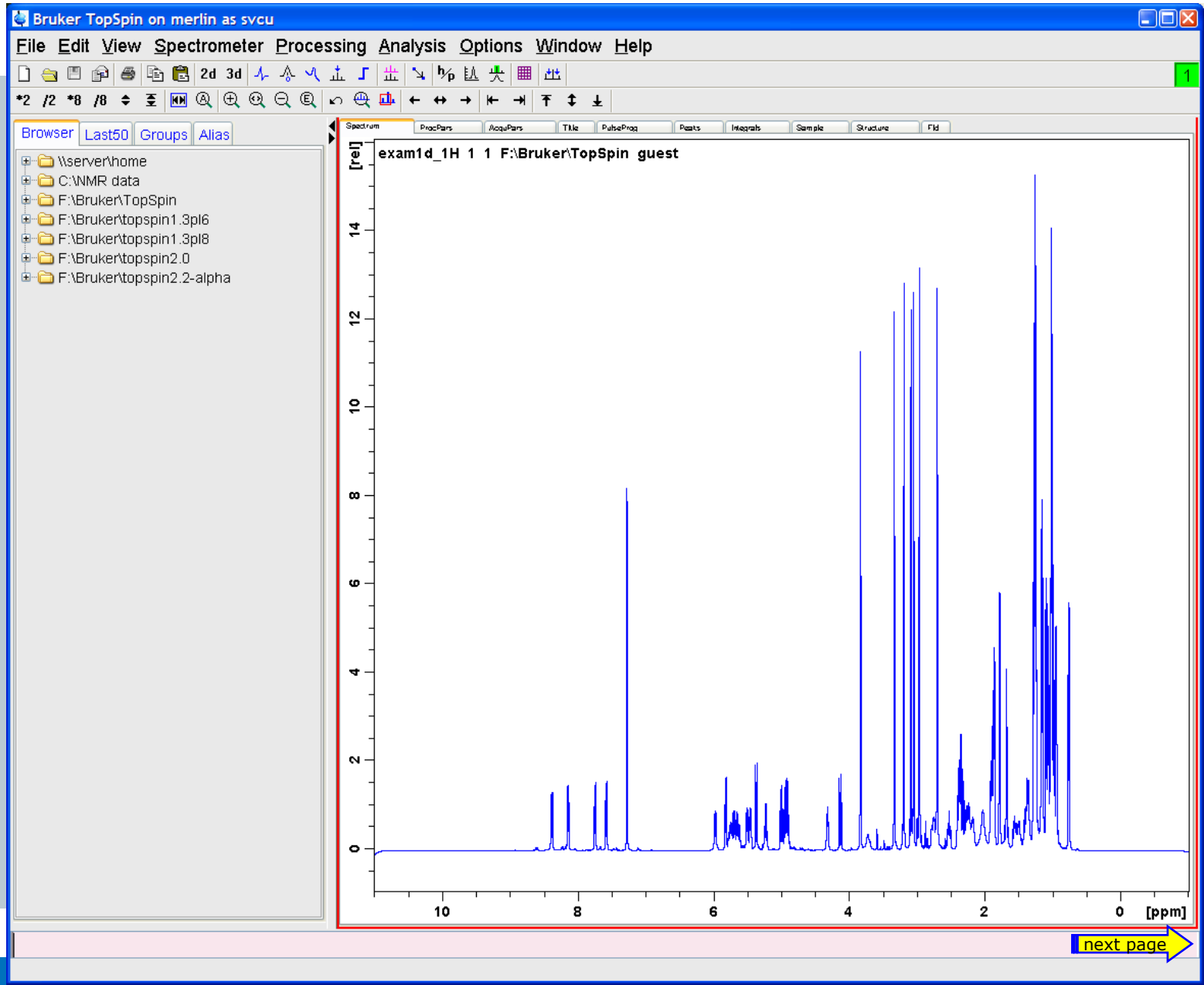

exam2d_HH 5 1 "C:\NMR data" tojd
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Fid
F1 [ppm]
F2 [ppm]
TopSpin 2.0
BRUKER
ProcPars
AcquPars
TopSpin 2.1
Peak picking complete. # Peaks found = 10
173

Content

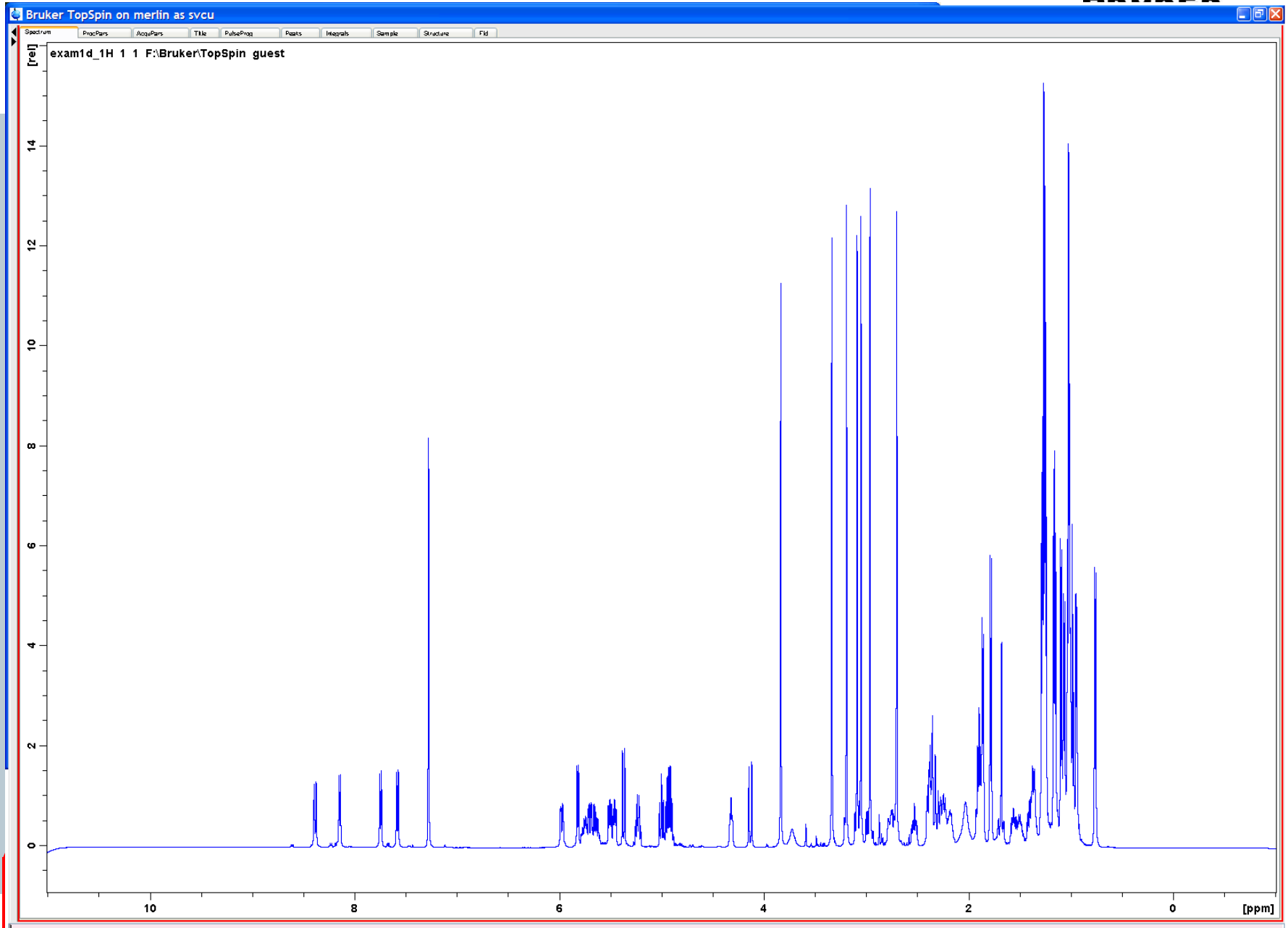

General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

New design of the TopSpin start window

New feature: **Toggle Window decoration**

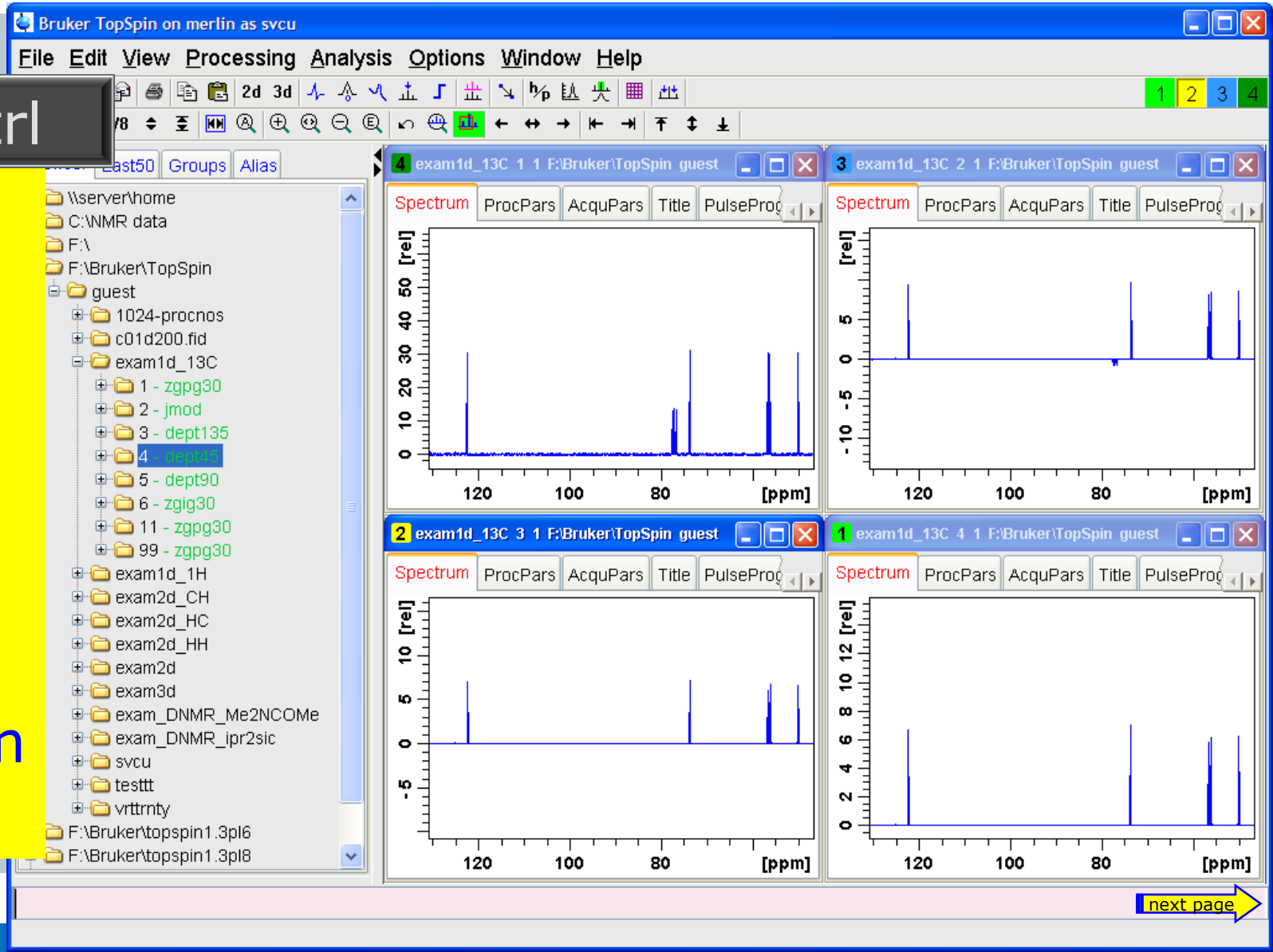


Even in Full screen mode available



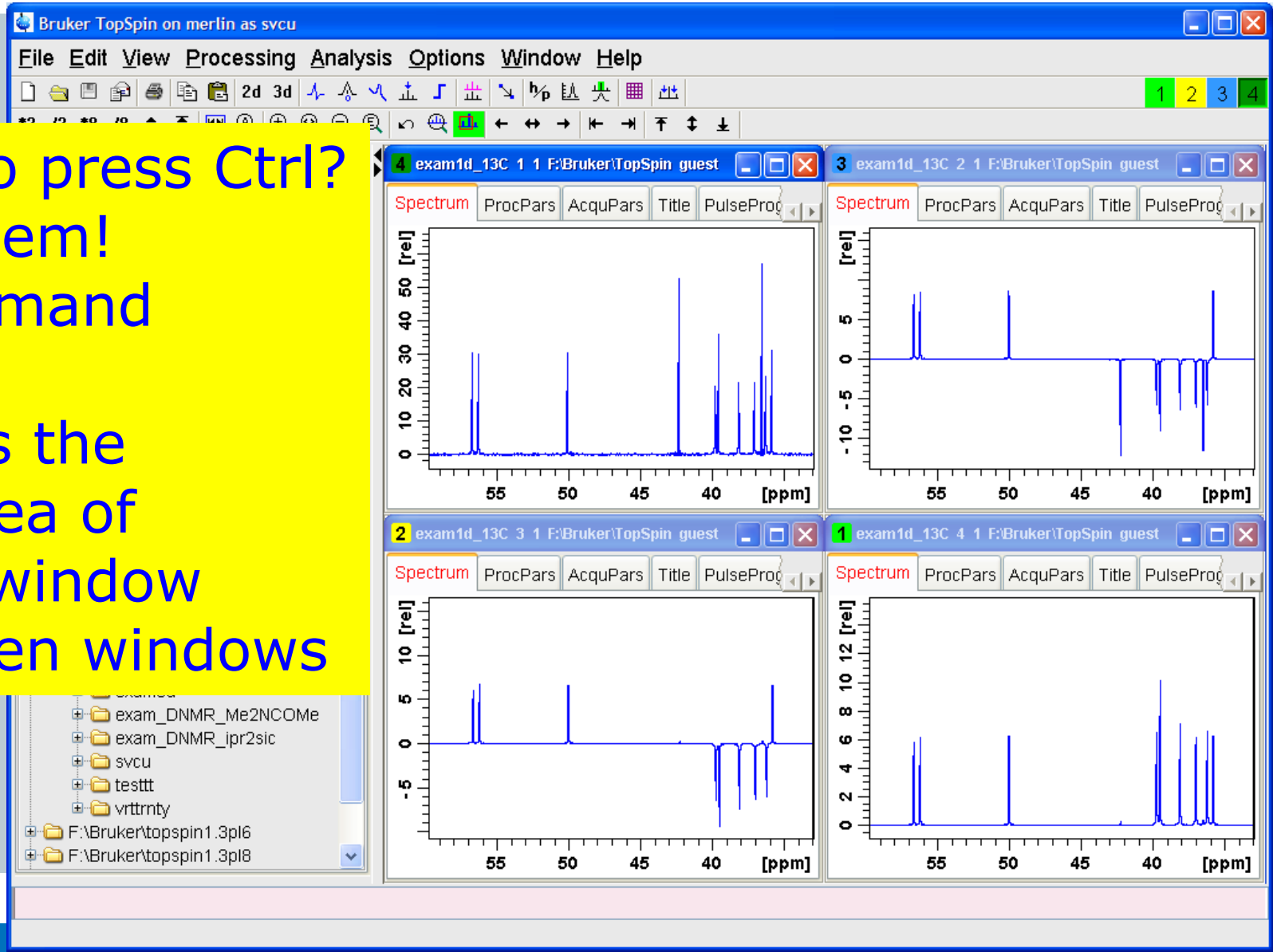
Zoom behaviour with multiple windows in TopSpin 2.1

press Ctrl key and keep it pressed ➔ all open datasets display same spectrum range



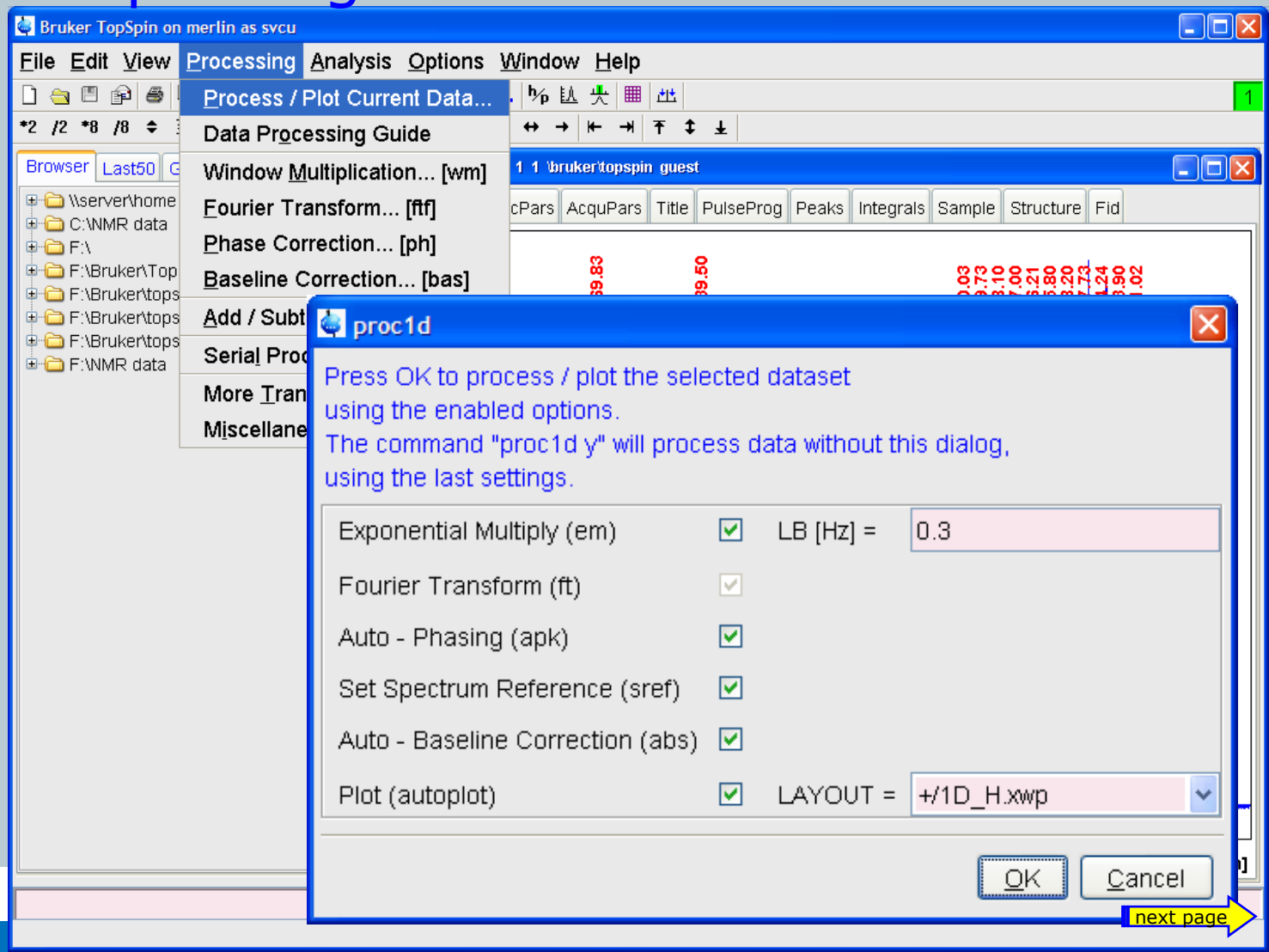
Zoom behaviour with multiple windows
TopSpin 2.1 – new command **.sync**

Forgot to press Ctrl?
No problem!
the command
.sync
transfers the
zoom area of
current window
to all open windows



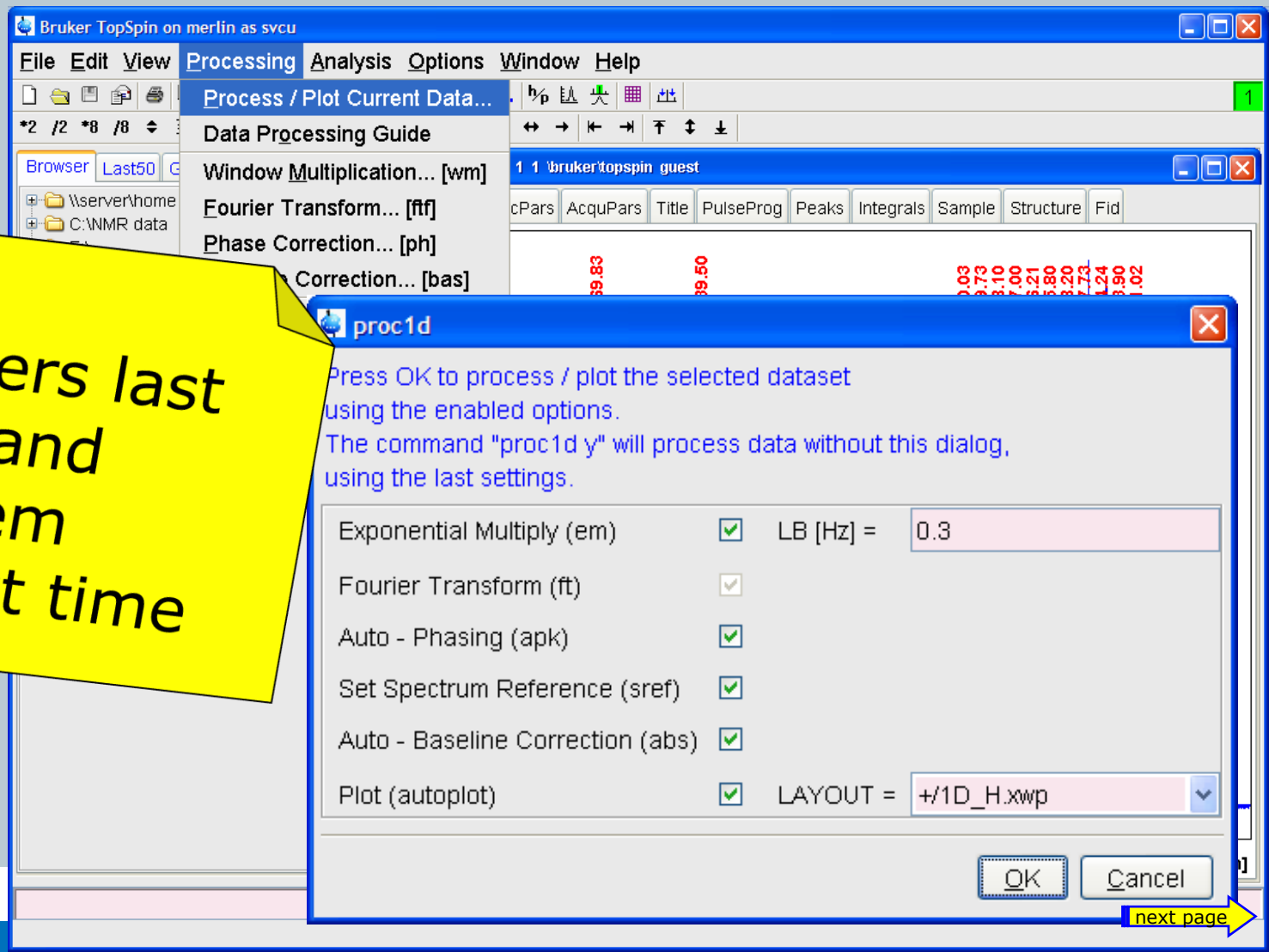
New command **proc1d**

proc1d offers a push-button solution for 1D processing and plotting



New command **proc1d**

proc1d offers a push-button solution for 1D processing

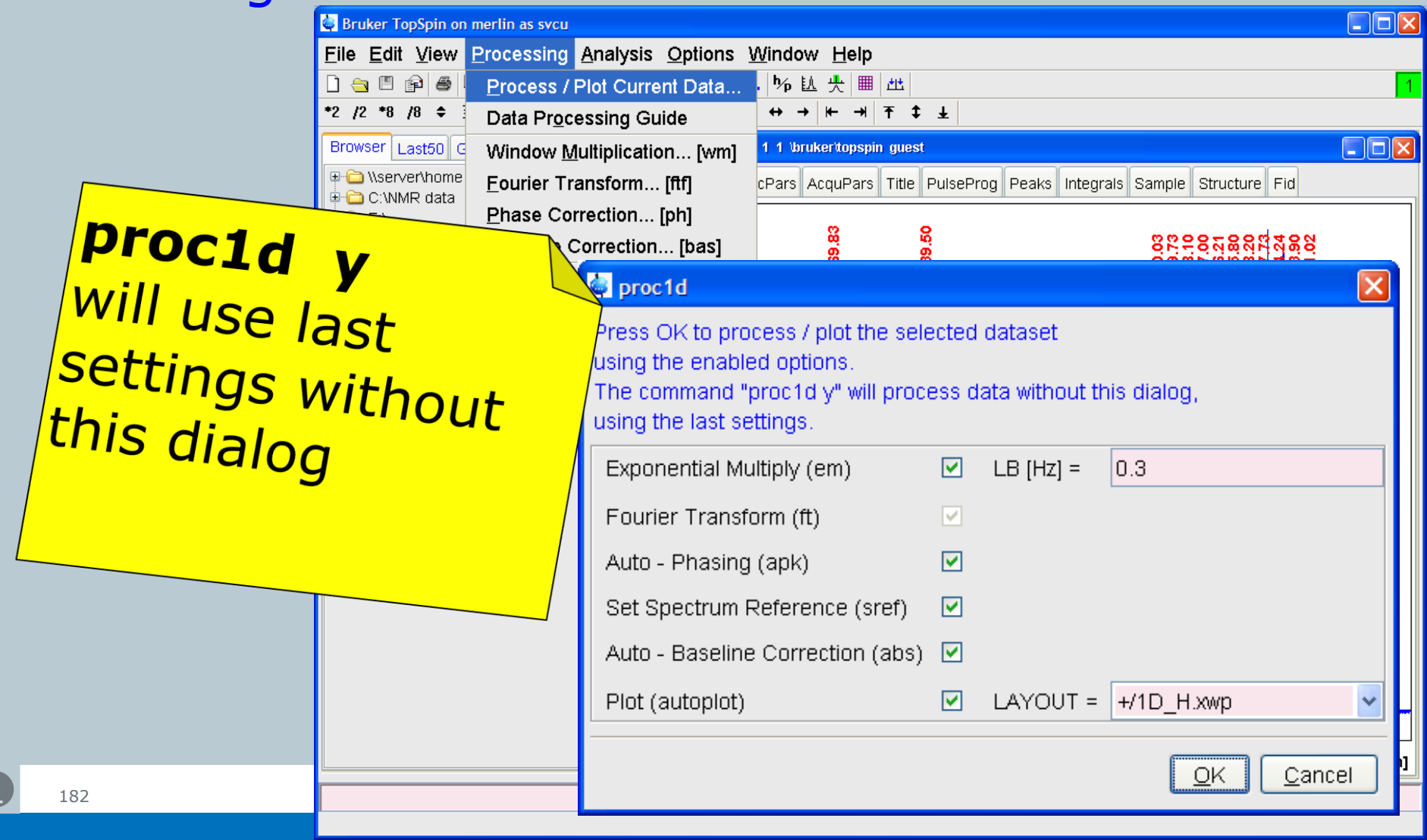


TopSpin remembers last settings and offers them again next time

next page

New command **proc1d**

proc1d offers a push-button solution for 1D processing

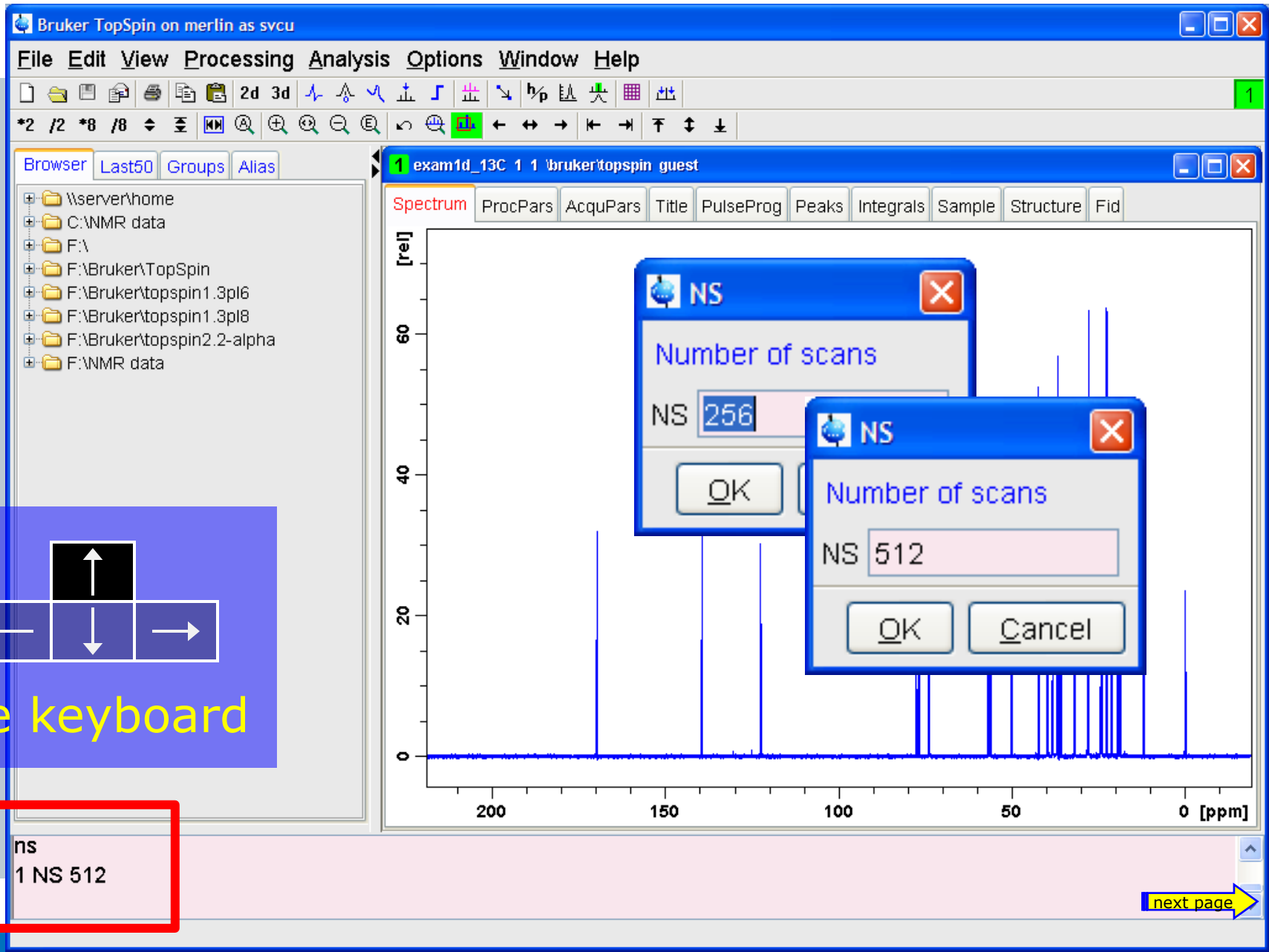


Command history

TopSpin command history
offers now the parameter
and its modified value,
even if it was not modified in the command line
but in the parameter window.

next page

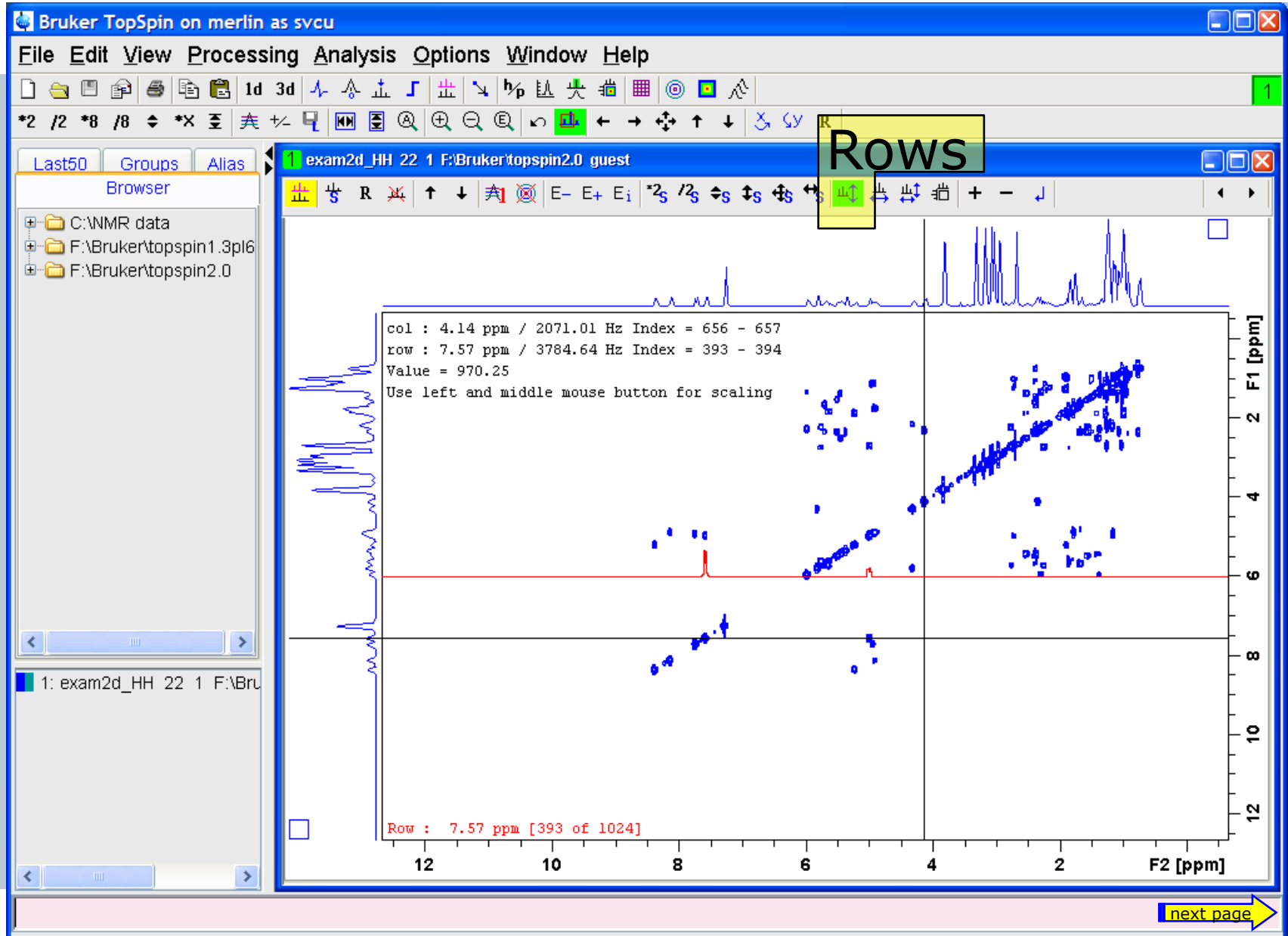
Command history



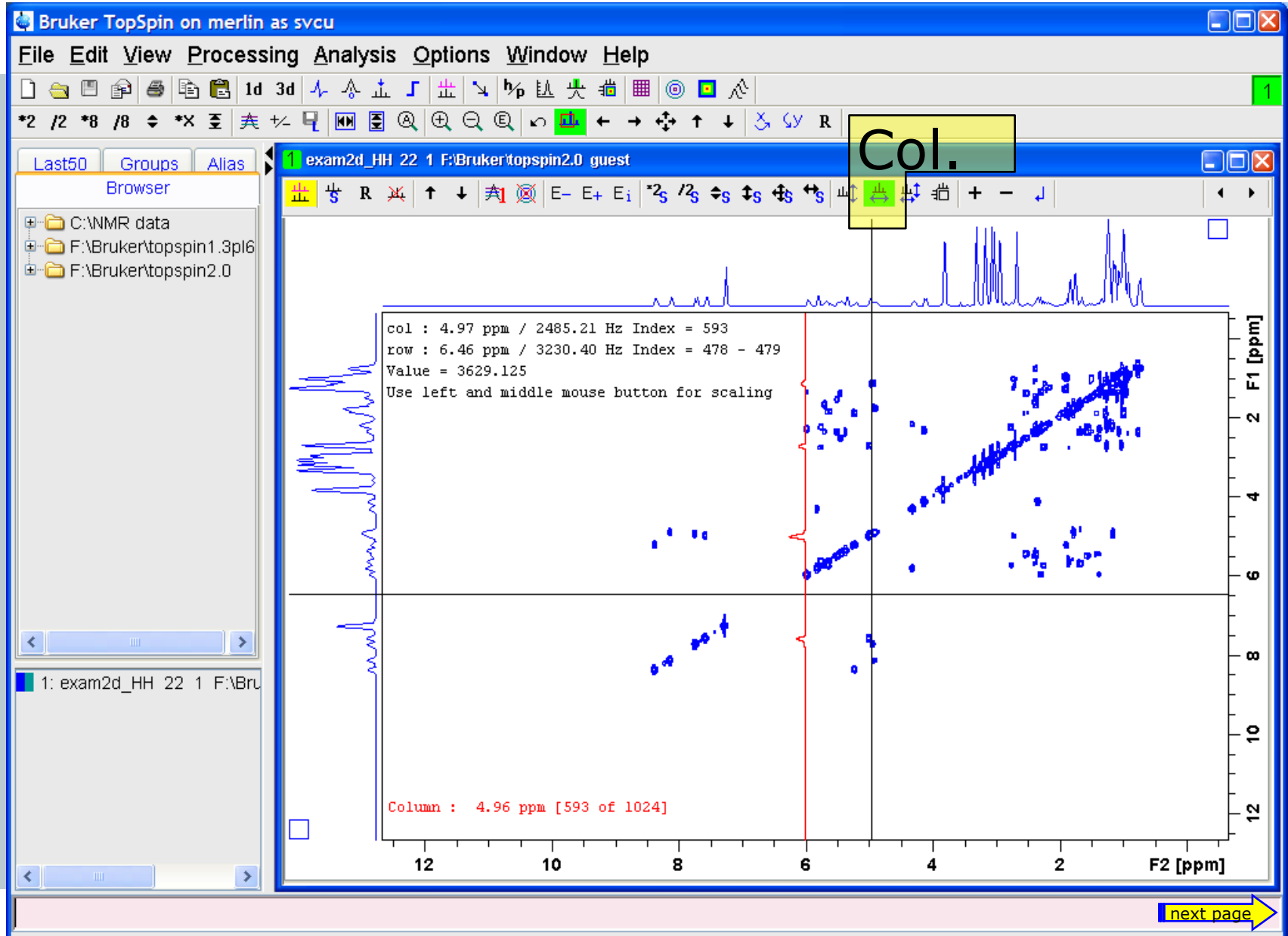
row/column scan

Now 2D multiple display allows scanning rows and columns simultaneously.

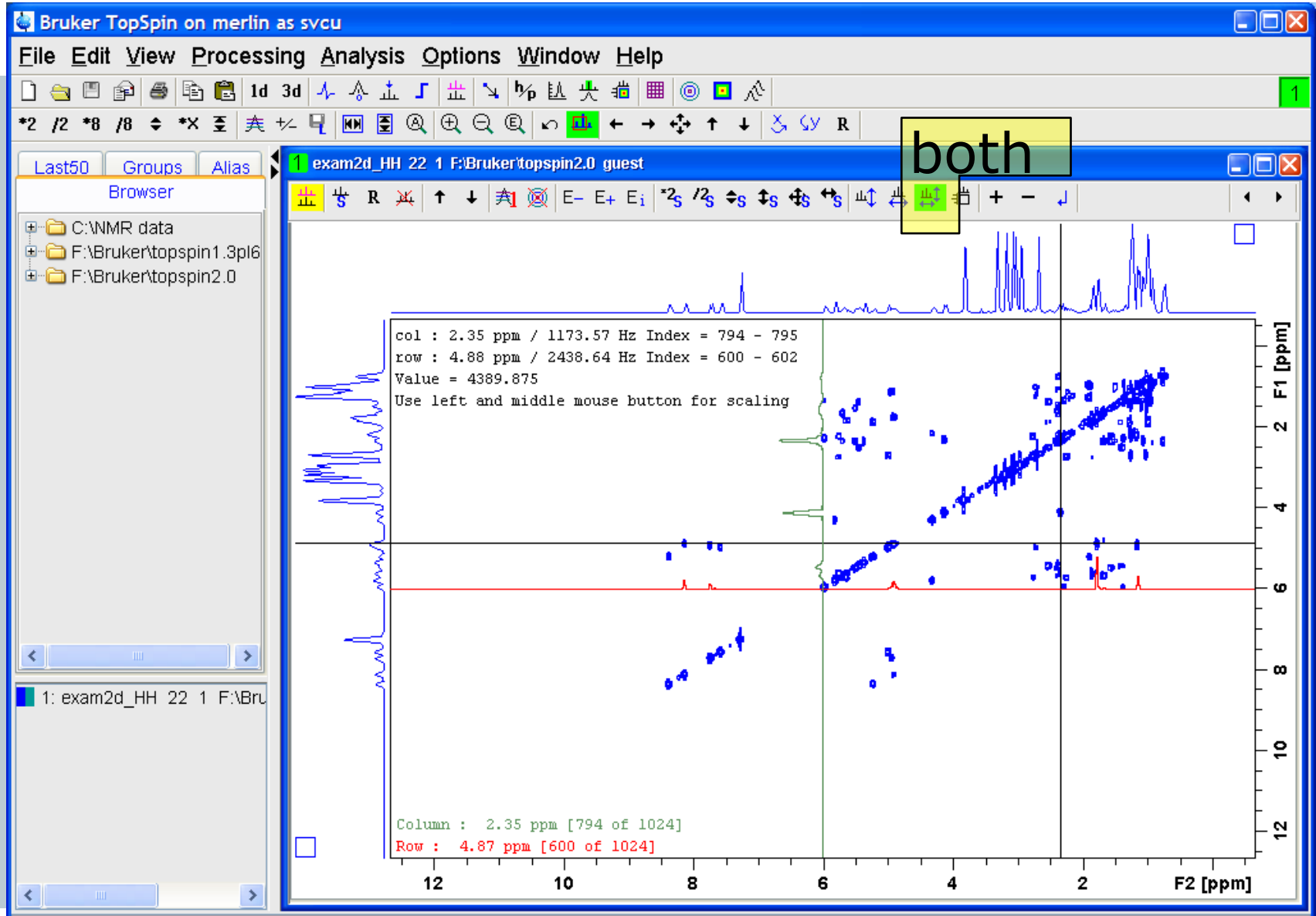
row/column scan



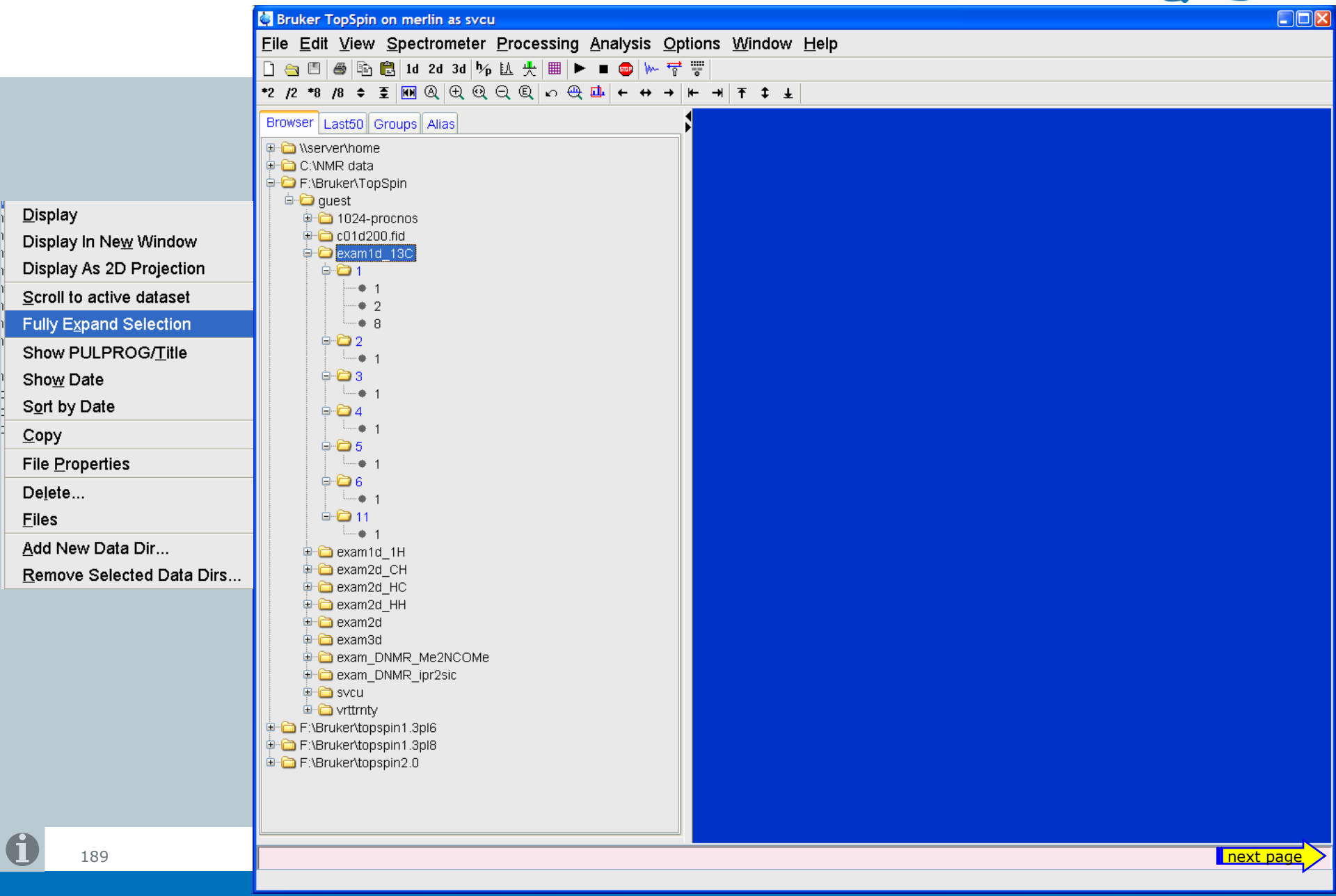
row/column scan



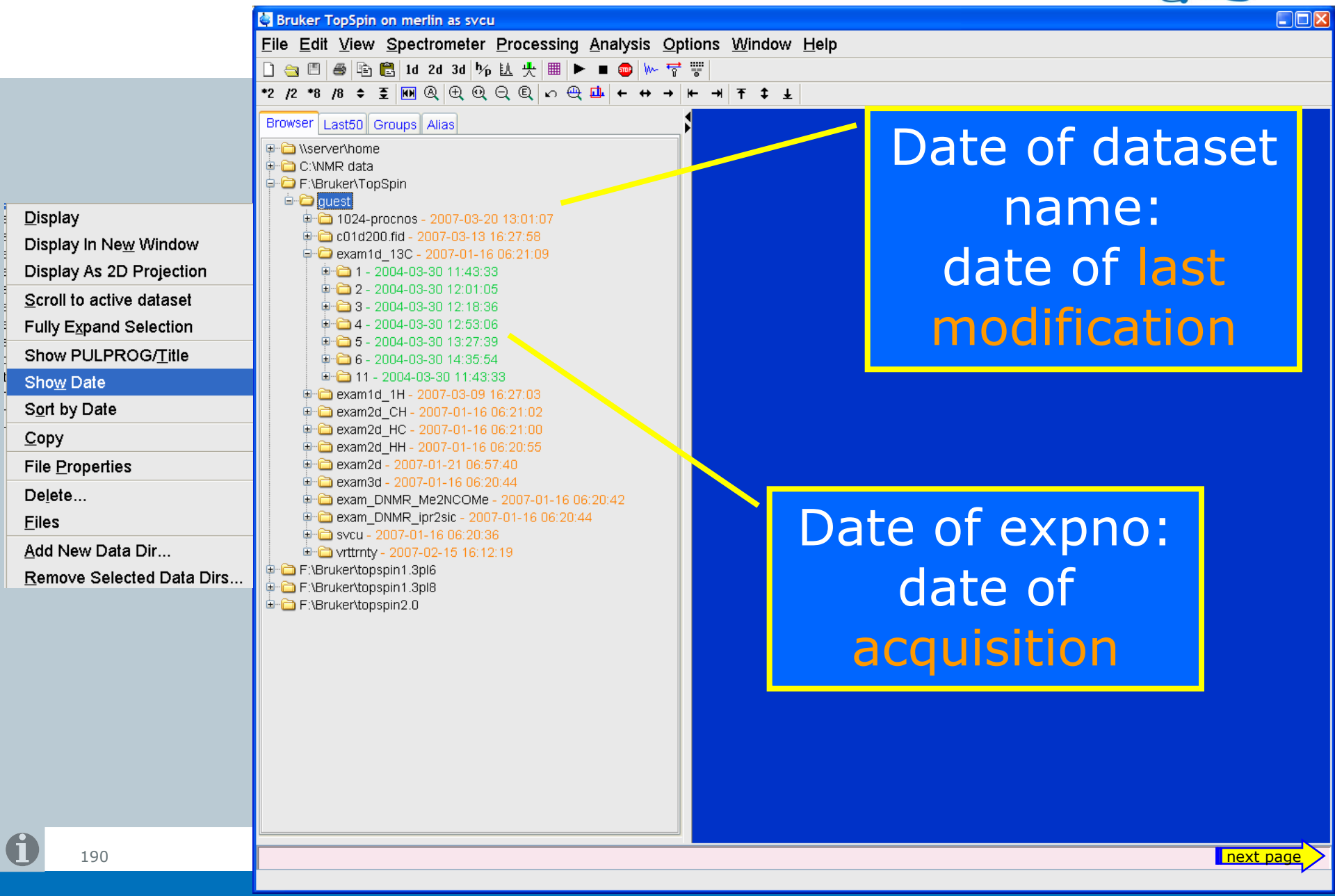
row/column scan



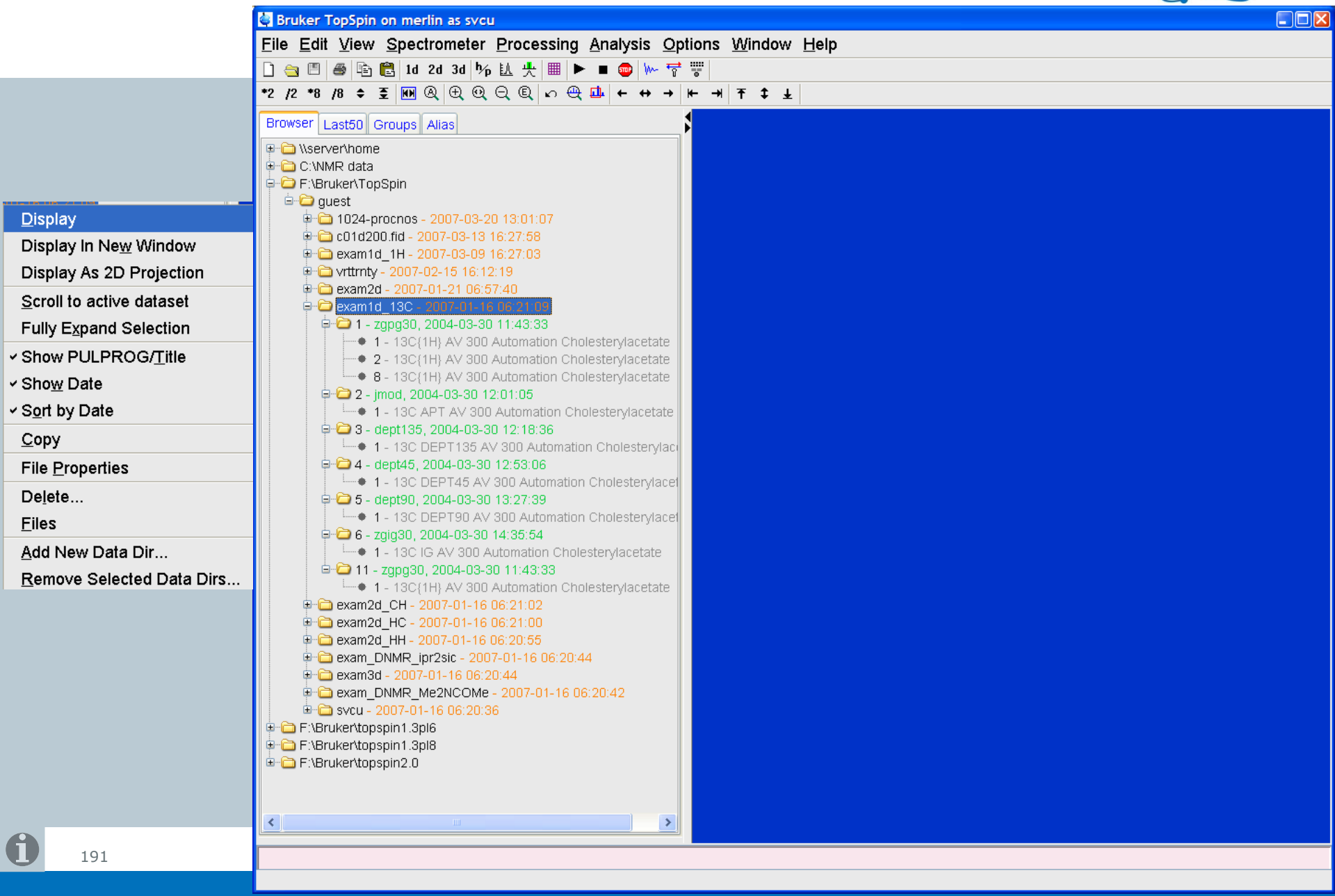
Browser: **Fully Expand Selection**



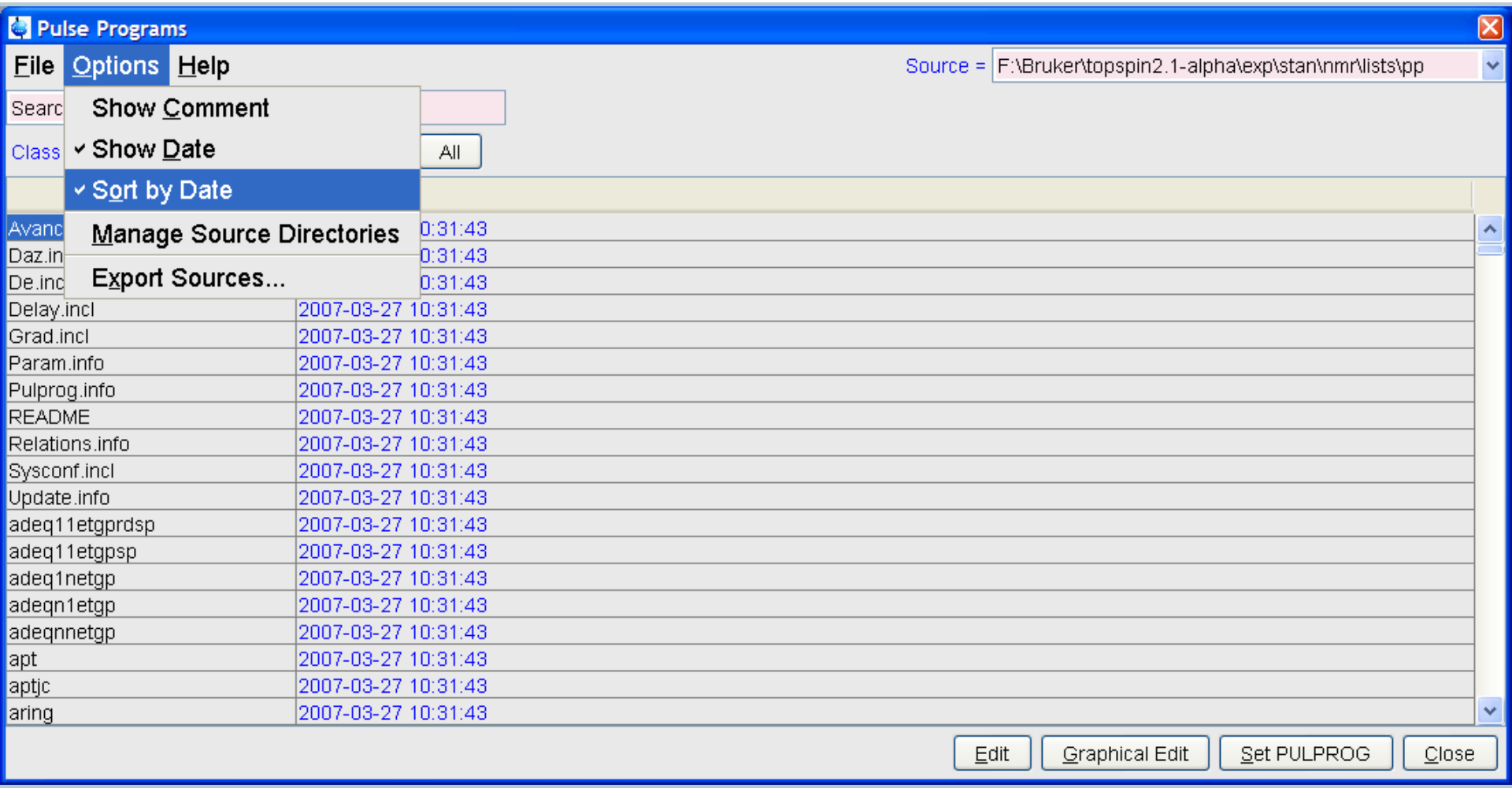
Browser: **Show Date**



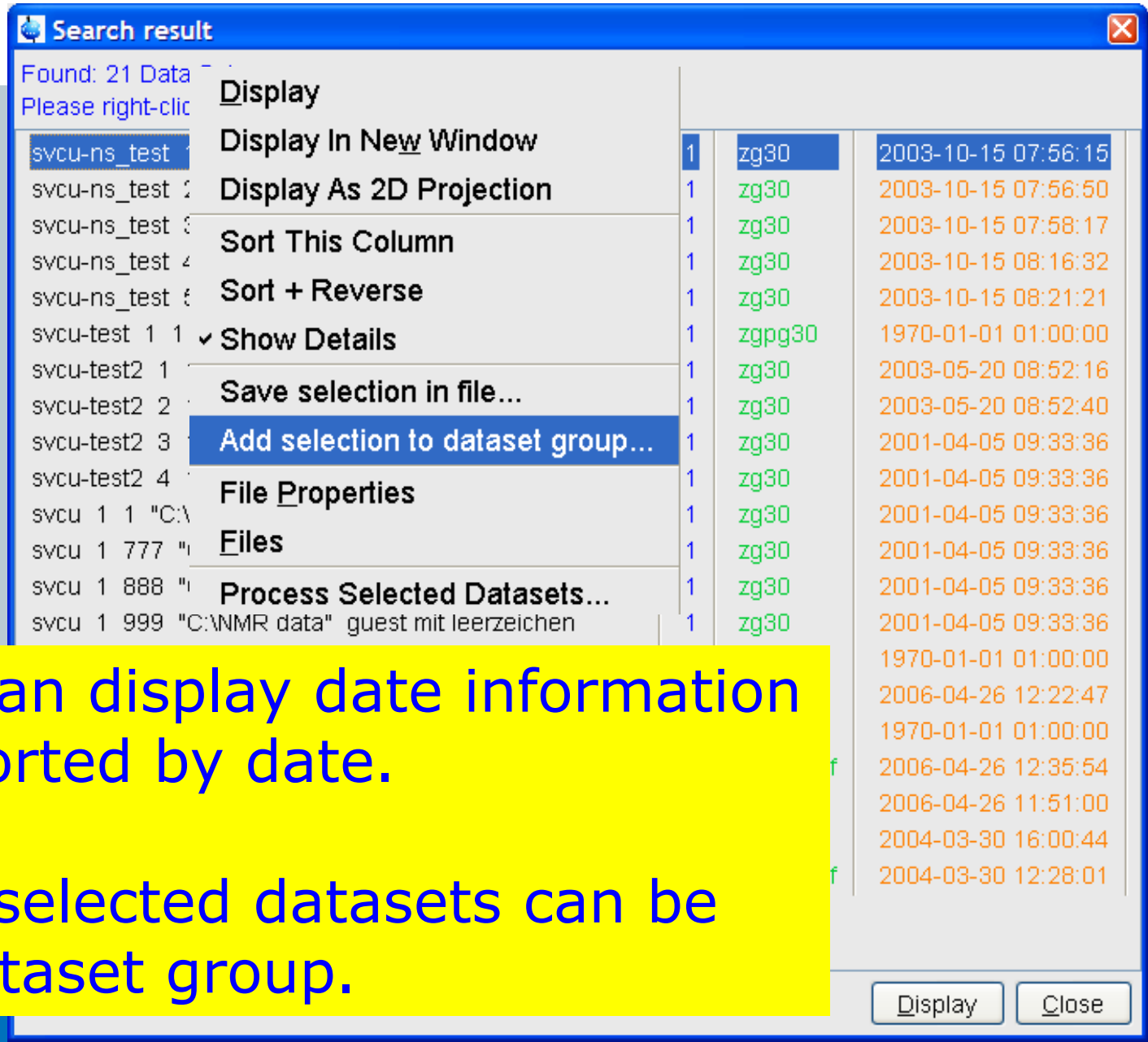
Browser: Date / Pulprog / Title



Sort by Date – e.g. **edpul**



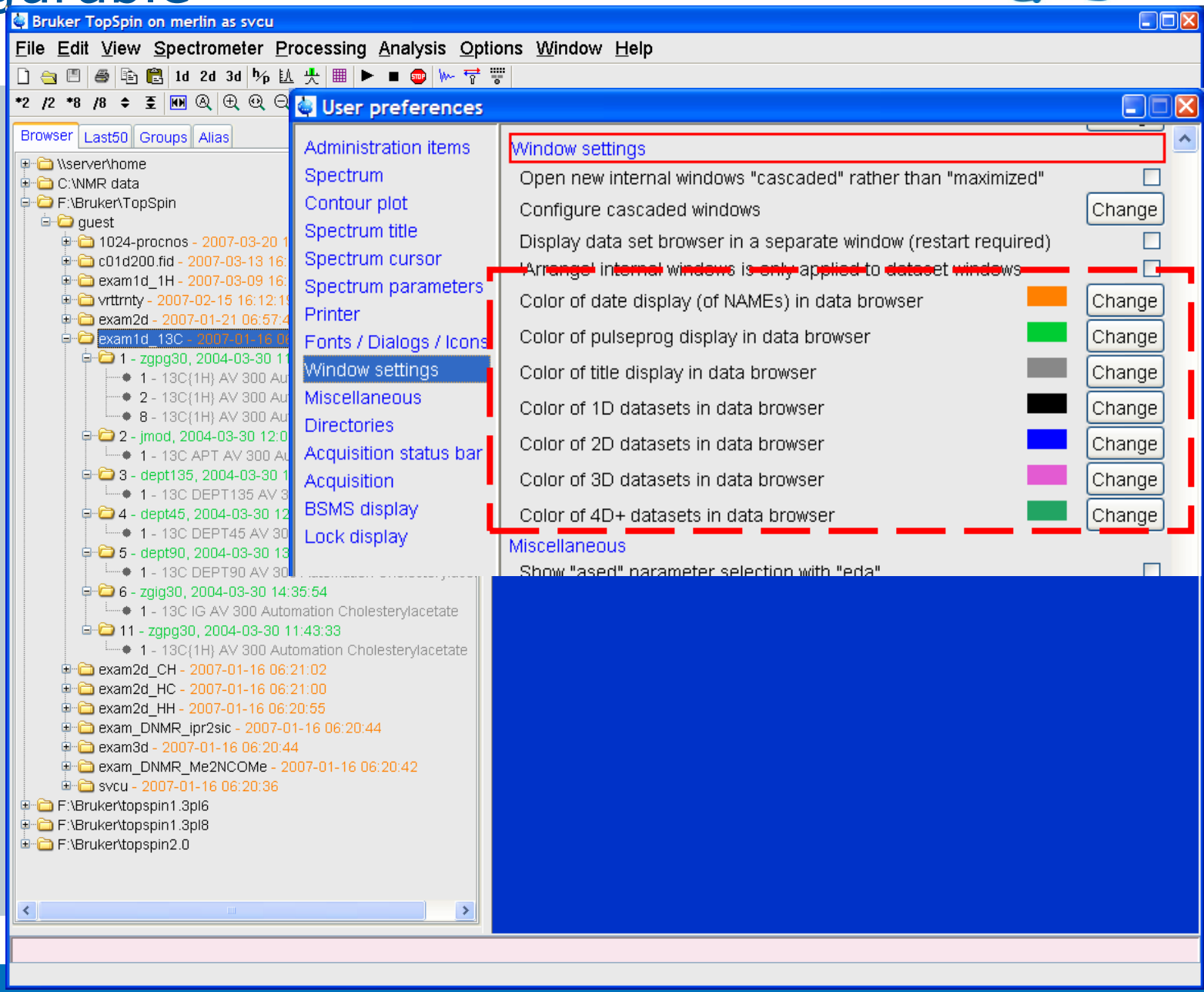
Search results



Find results can display date information and can be sorted by date.

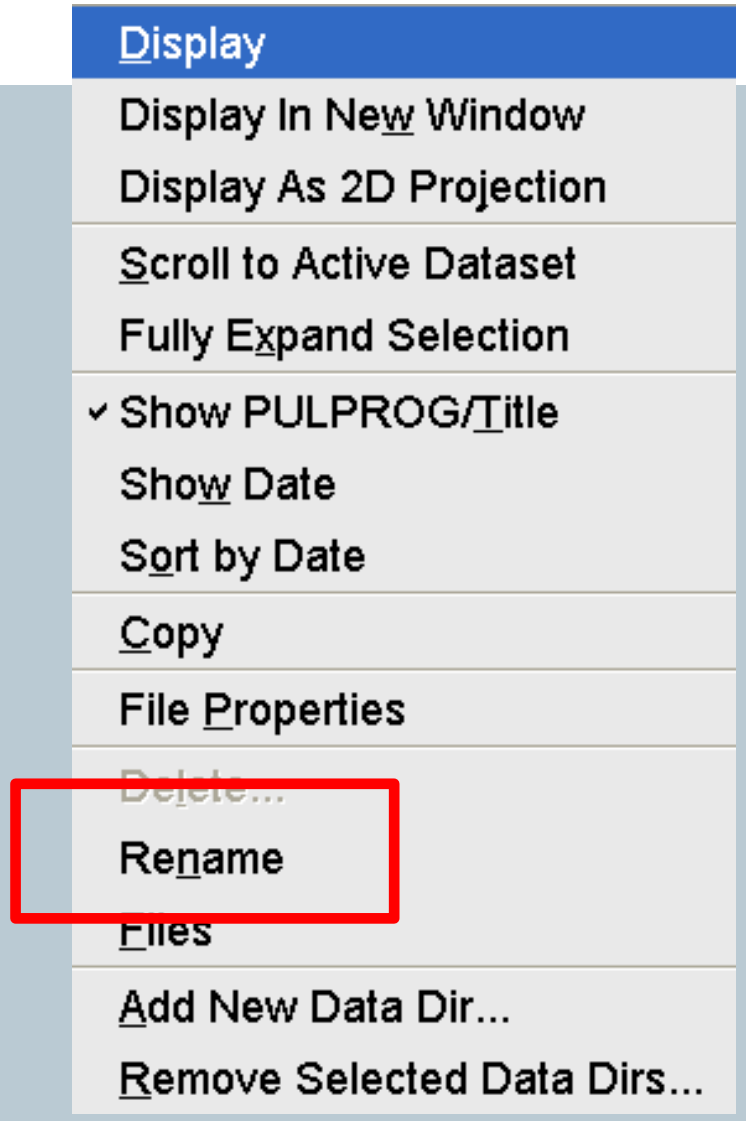
Furthermore selected datasets can be defined as dataset group.

Colours of additional information are configurable



TopSpin databrowser offers '**Rename**'

TopSpin data browser allows renaming of Names, Expnos or Procnos.

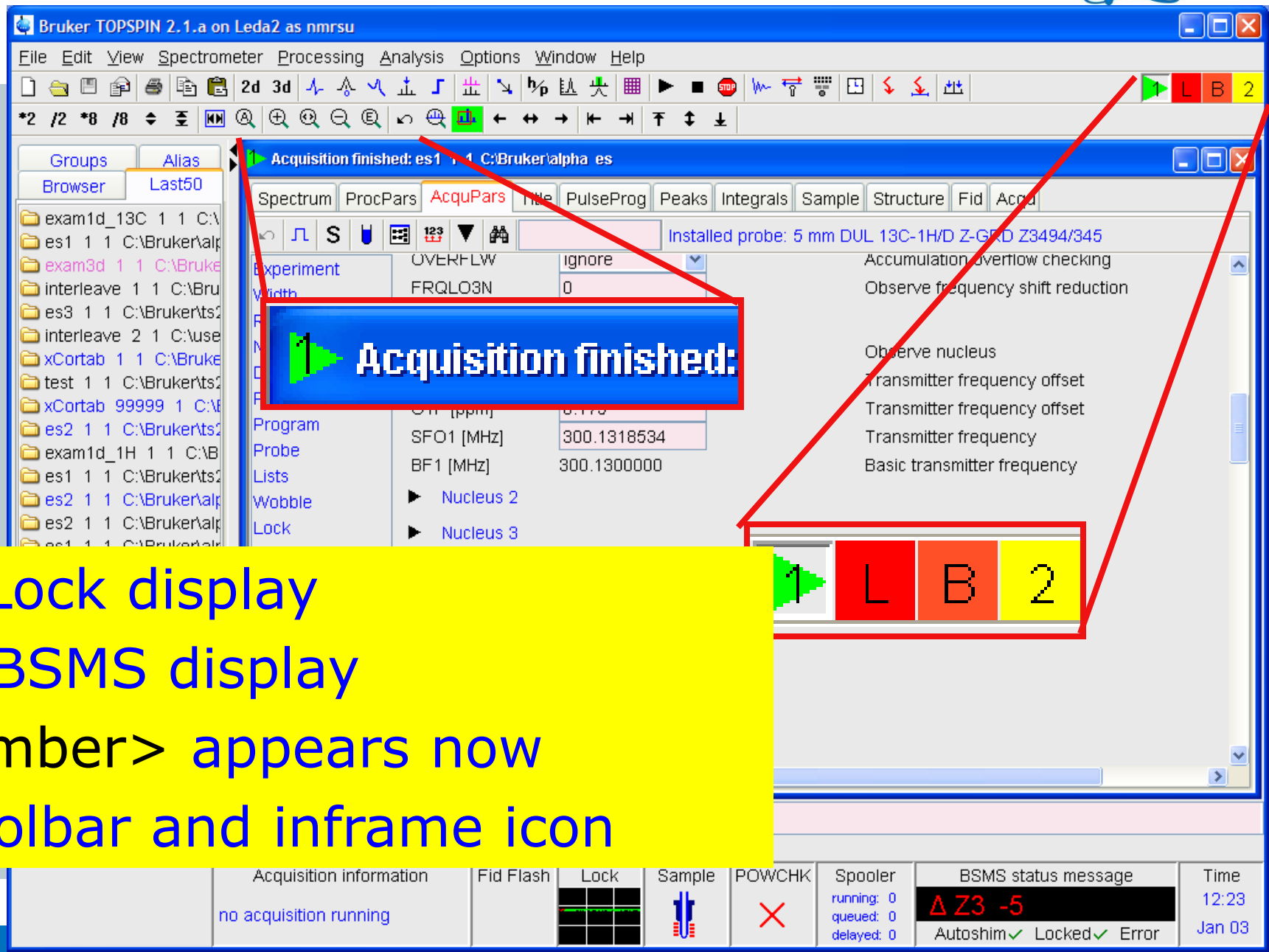


Drag&Drop from TopSpin databrowser can be turned off

Drag&Drop of datasets into TopSpin main window can now be disabled.
This is useful is this functionality leads to any problems like a graphics hangup.
For details see respective FAQ in the Bruker Knowledge Base, item #7222:

http://www.bruker-biospin.com/shell/bkb/show_bug.cgi?id=7222

Window numbering

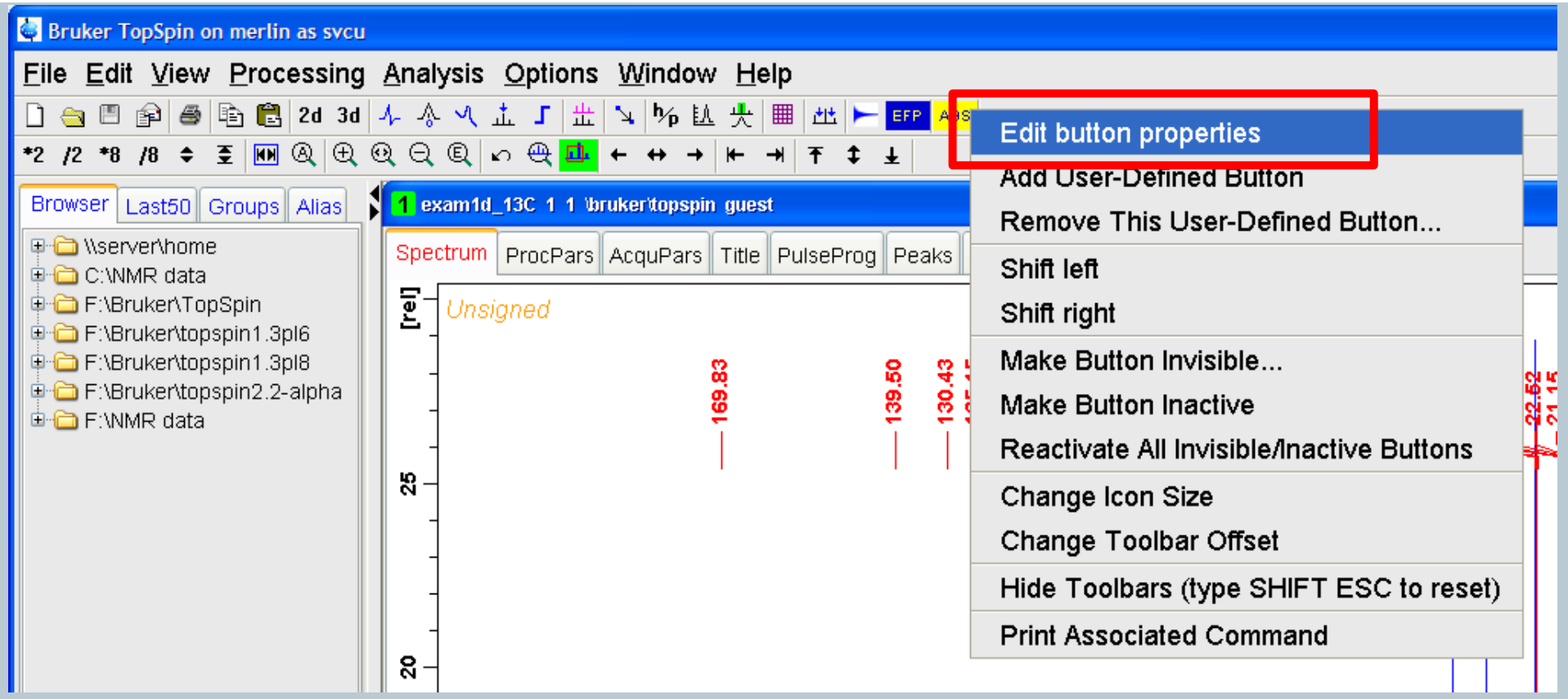


L = Lock display

B = BSMS display

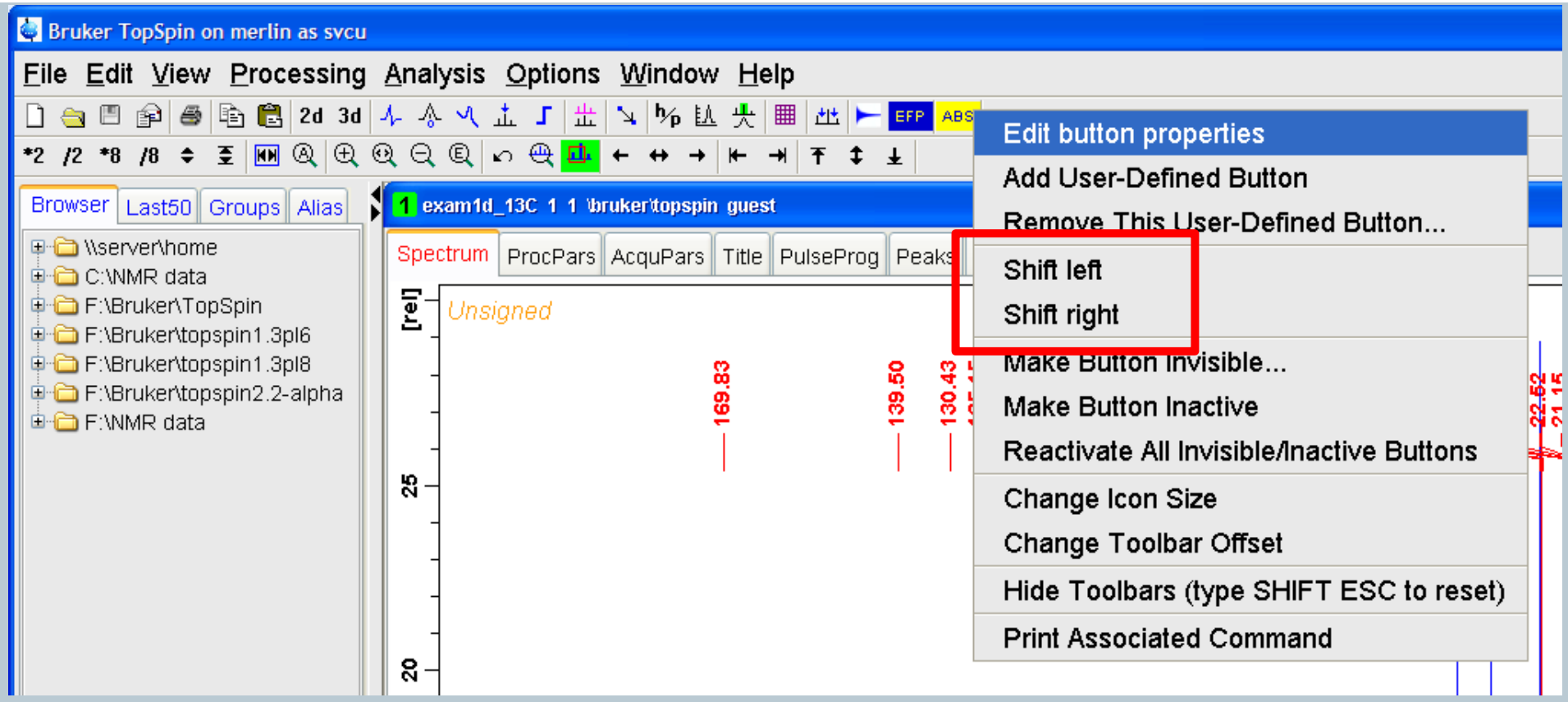
<number> appears now in toolbar and inframe icon

User-specific icons can now be edited

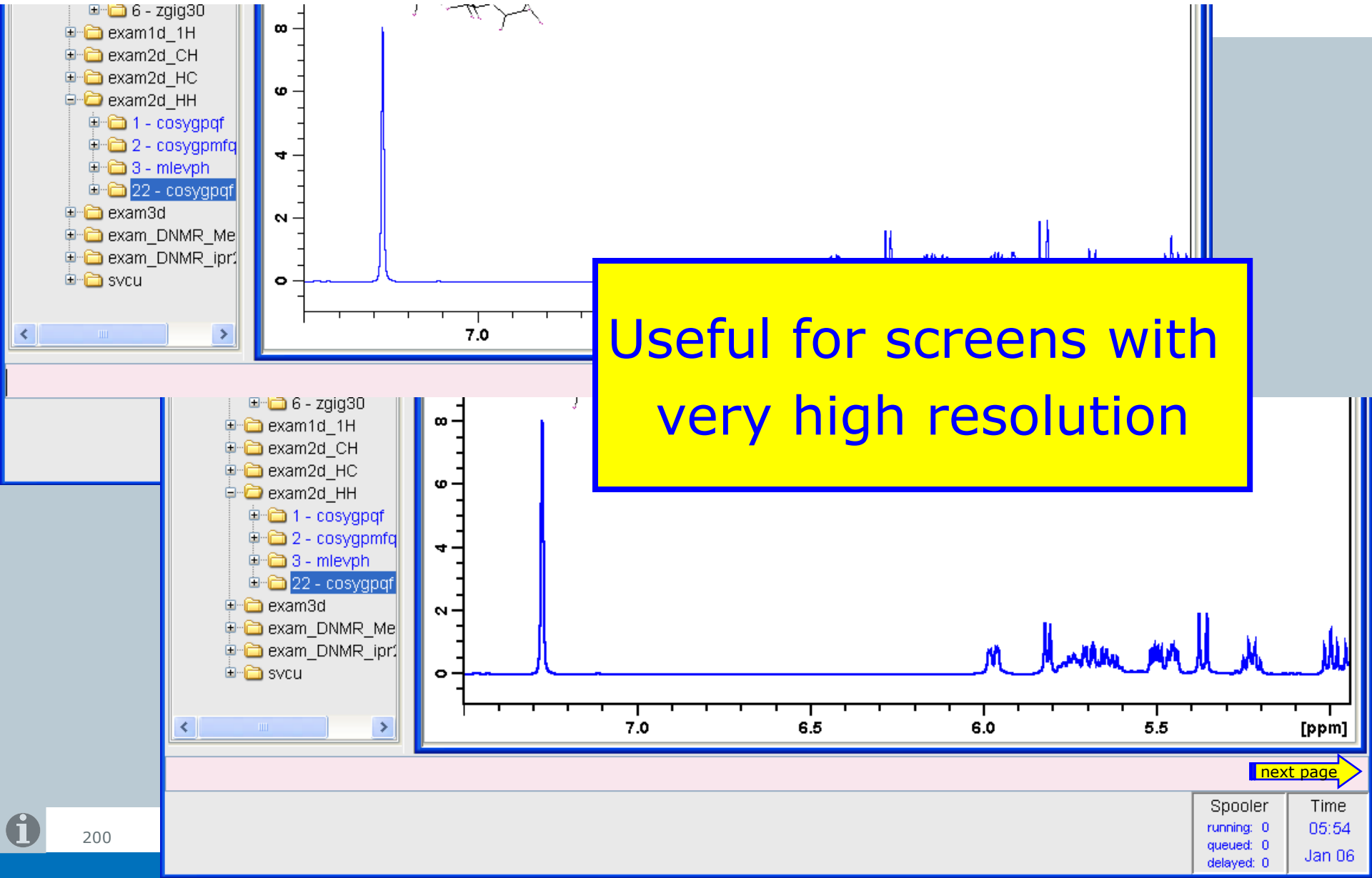


next page

User-specific icons can now be edited and shifted to another position



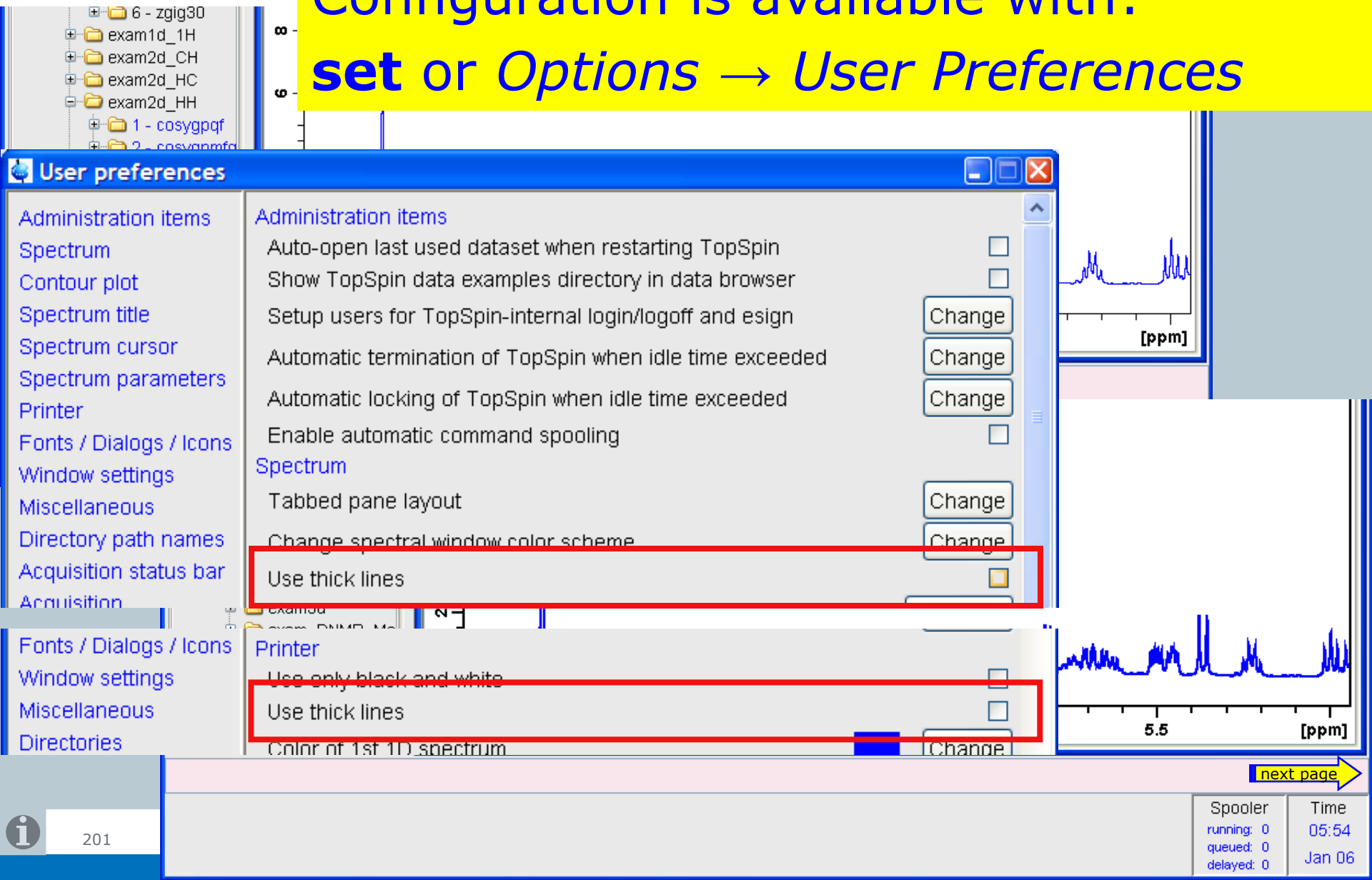
Thick spectra lines



Thick spectra lines

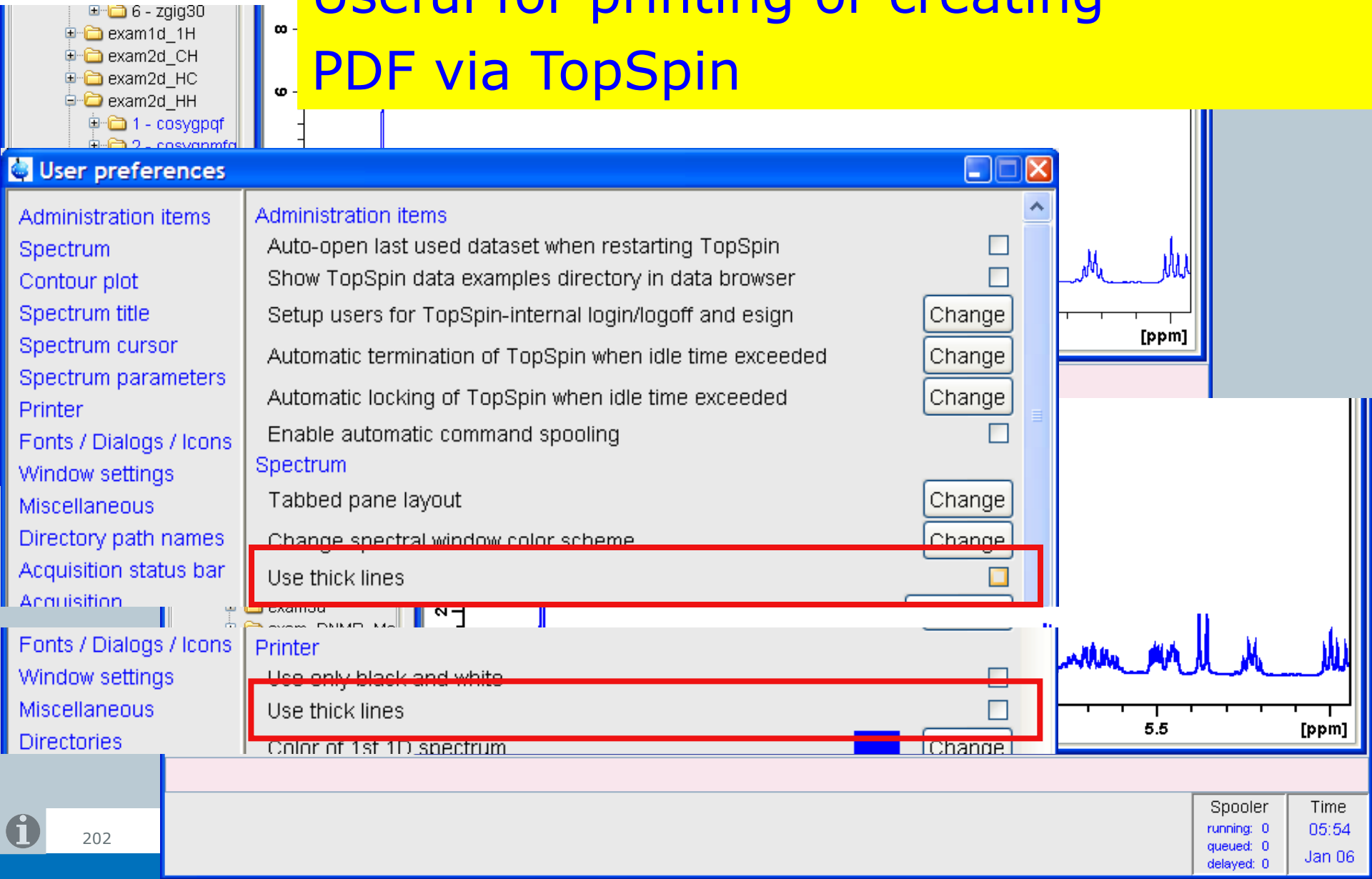
Configuration is available with:

set or *Options → User Preferences*

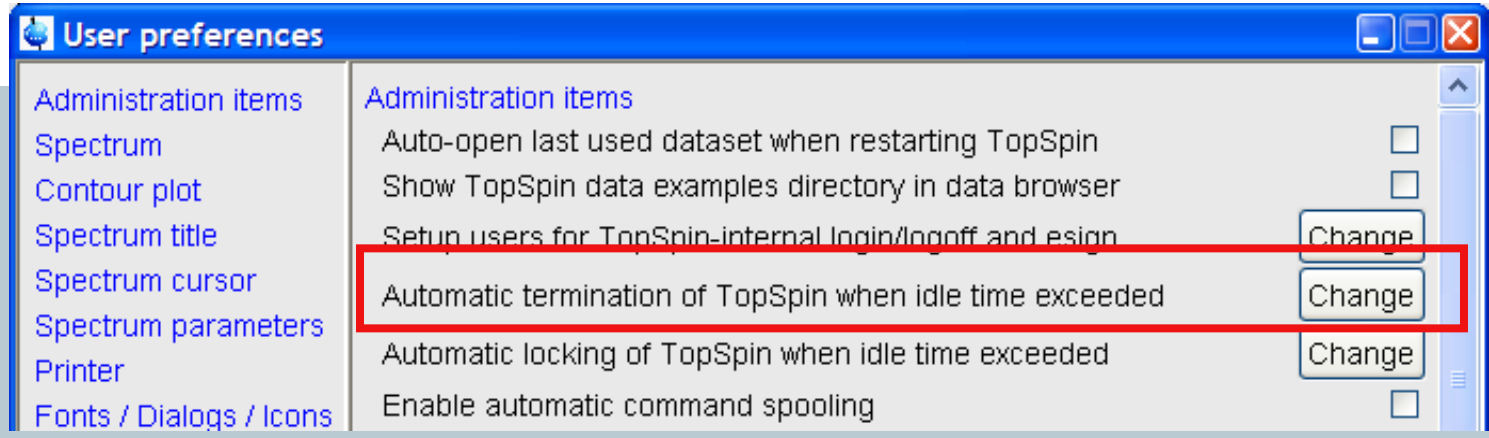


Thick spectra lines

Useful for printing or creating PDF via TopSpin



Thick spectra lines



Idle time for automatic termination of TopSpin can be configured globally for all users.

More details can be found in the Bruker Knowledge Base item

http://www.bruker-biospin.com/shell/bkb/show_bug.cgi?id=7236

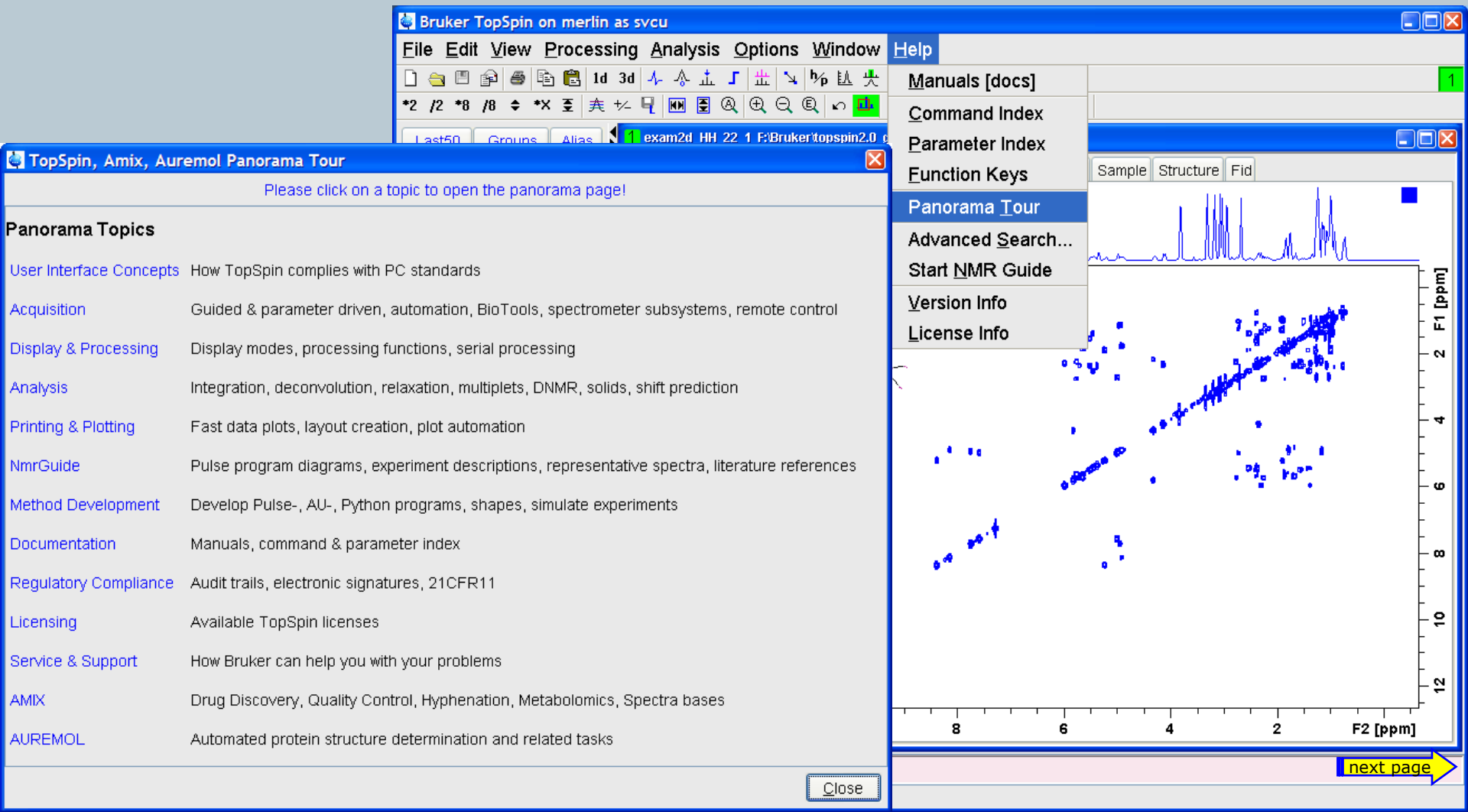
Seize/Font of TopSpin tabs

The desired font for the tabs can now be configured within *User* → *Preferences*

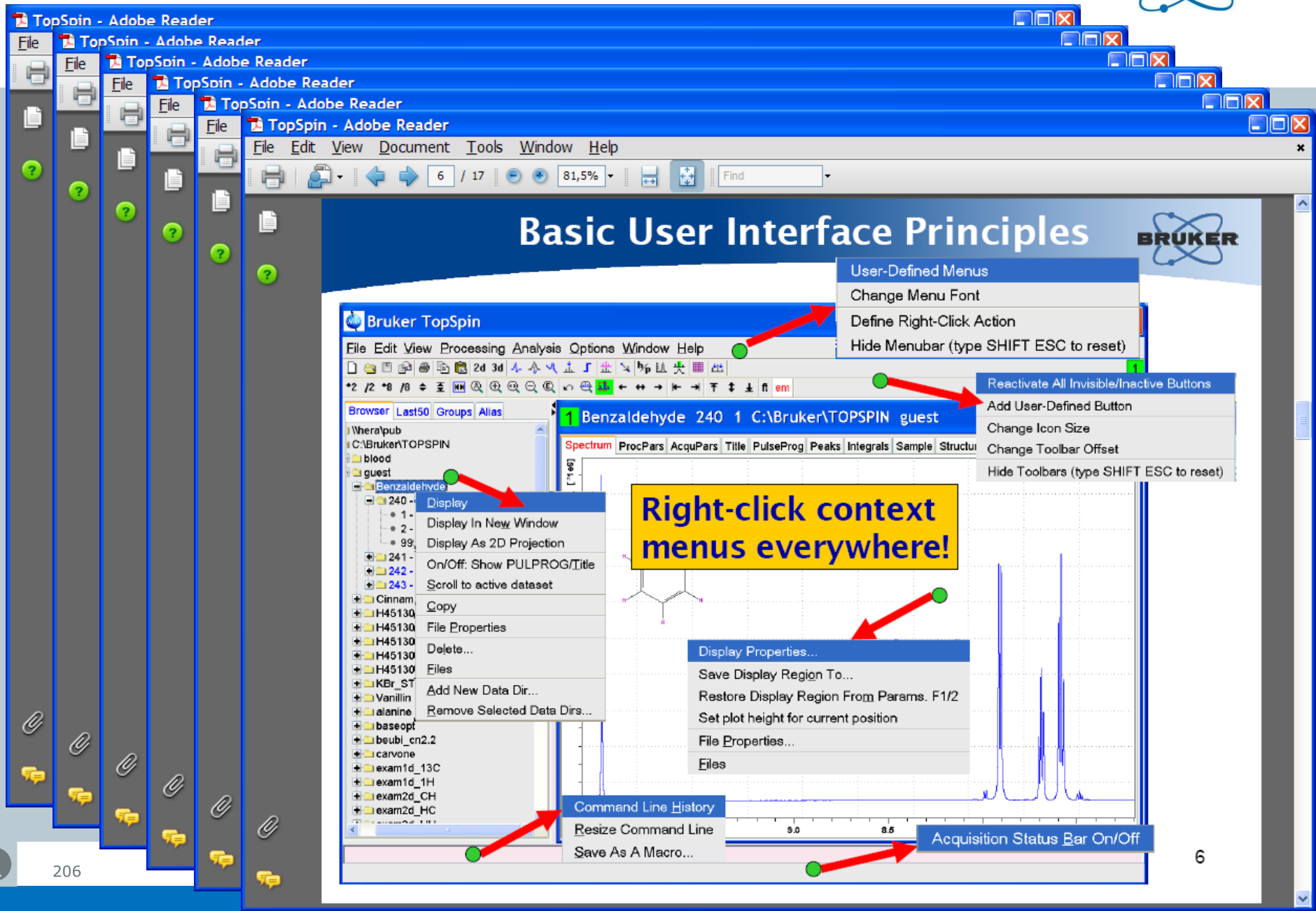
The height of the tabs corresponds to the height of the icon size, which can also be configured within *User* → *Preferences*

TopSpin Panorama Tour

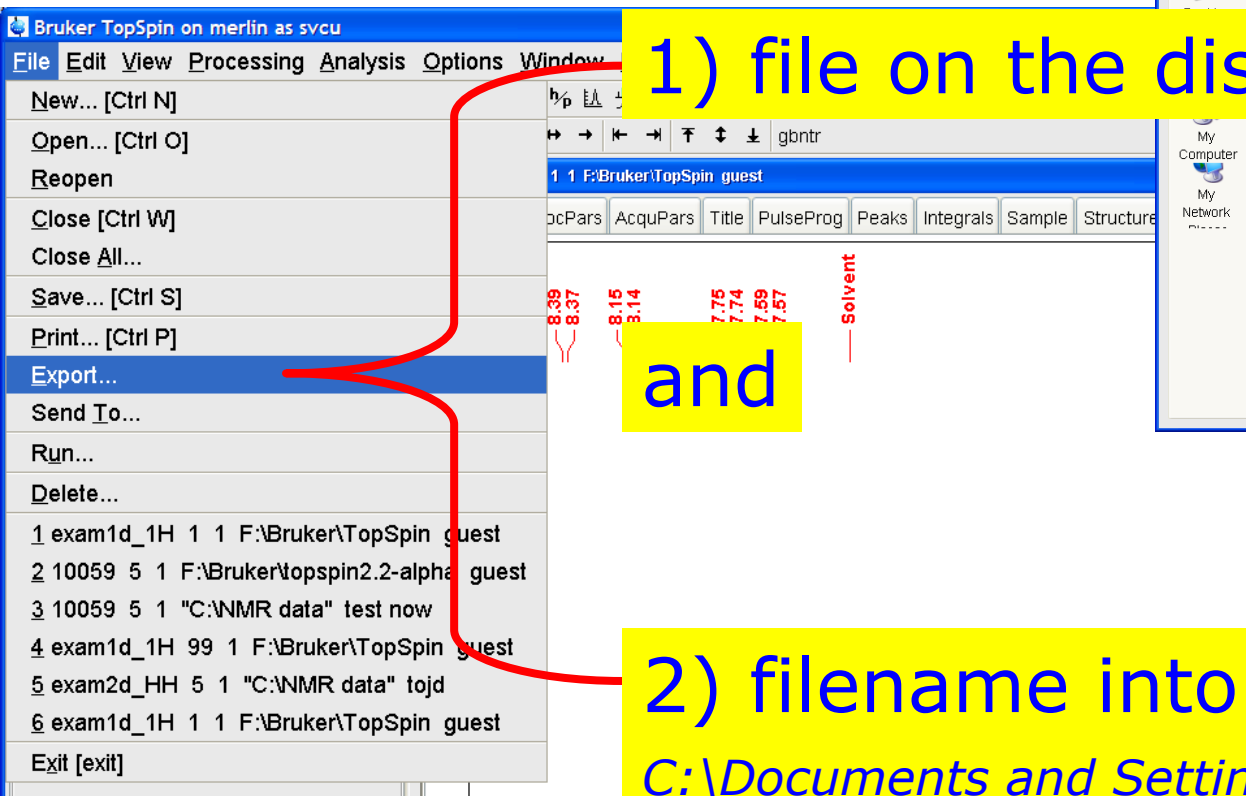
A short overview about some special TopSpin topics:



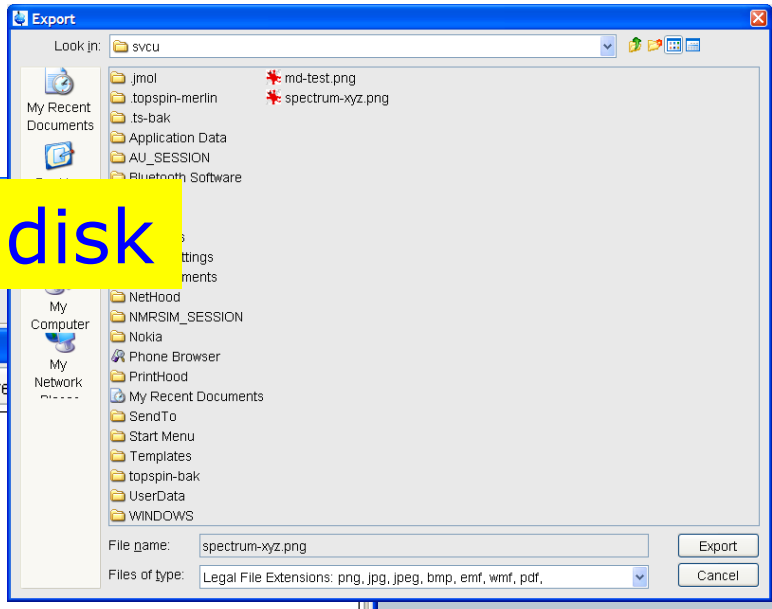
TopSpin Panorama Tour



Filename of exported picture available in clipboard



1) file on the disk



and

2) filename into clipboard

C:\Documents and Settings\svcu\spectrum-xyz.png

Bruker BioSpin

Windows: New format for command Copy

On Windows systems:

copy now stores in bmp format

The new command

copy wmf

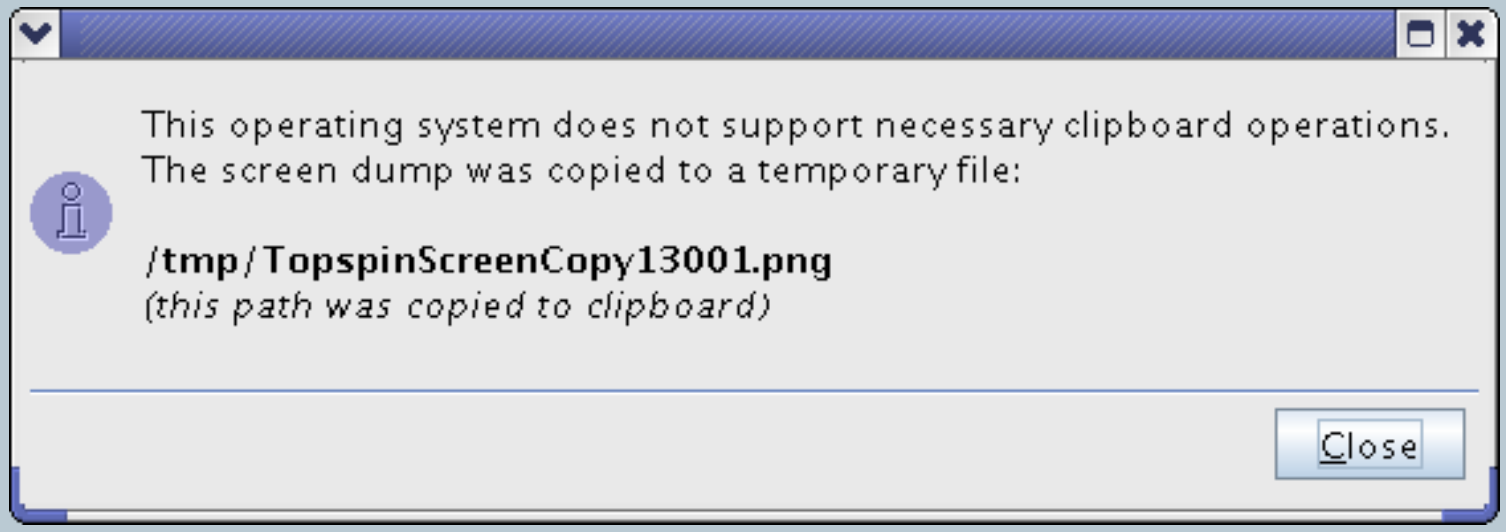
stores wmf format, which was the default format in previous TopSpin versions

Linux: Copy can now be used

On Linux systems:

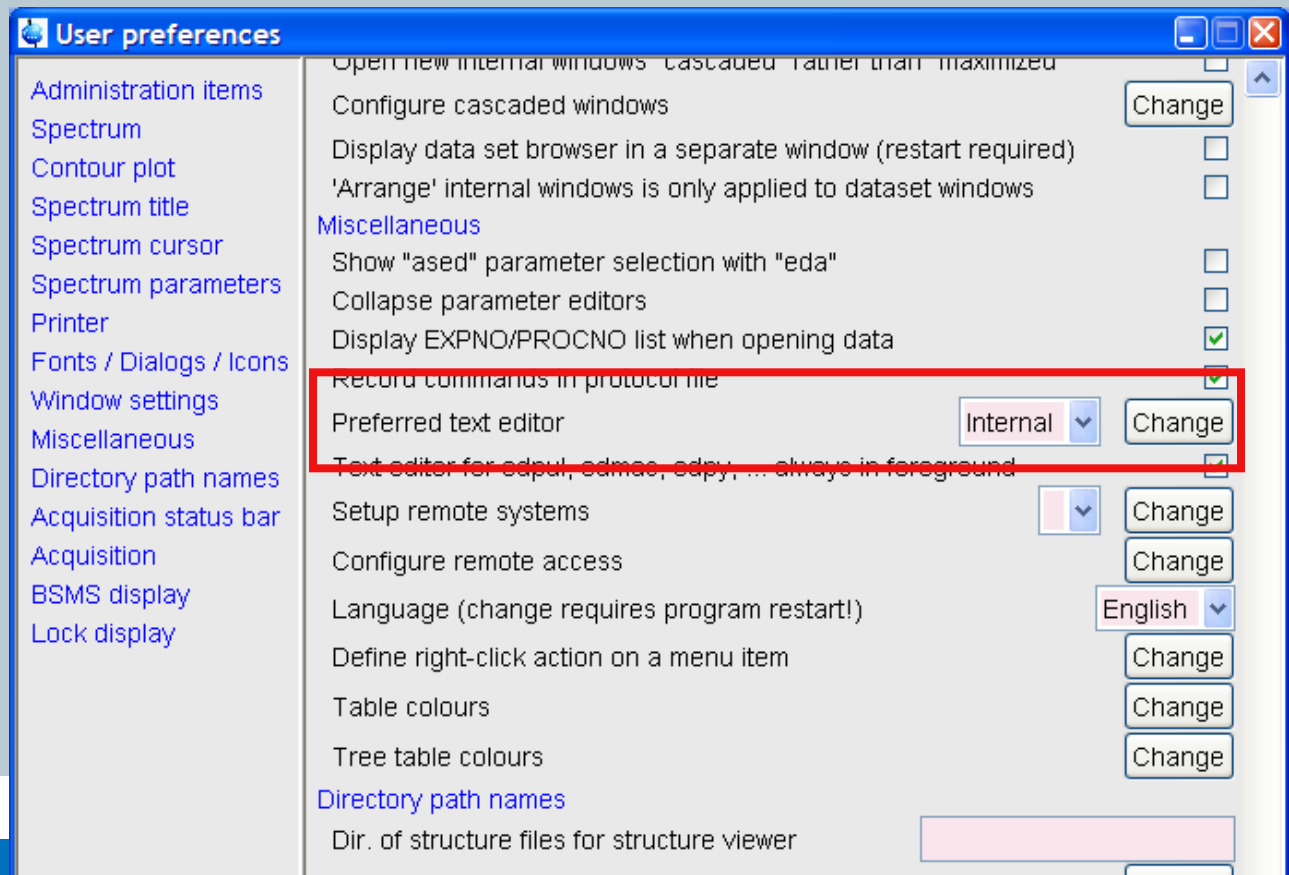
Copy stores png format into a temporary file,

the pathname of this file is copied to clipboard



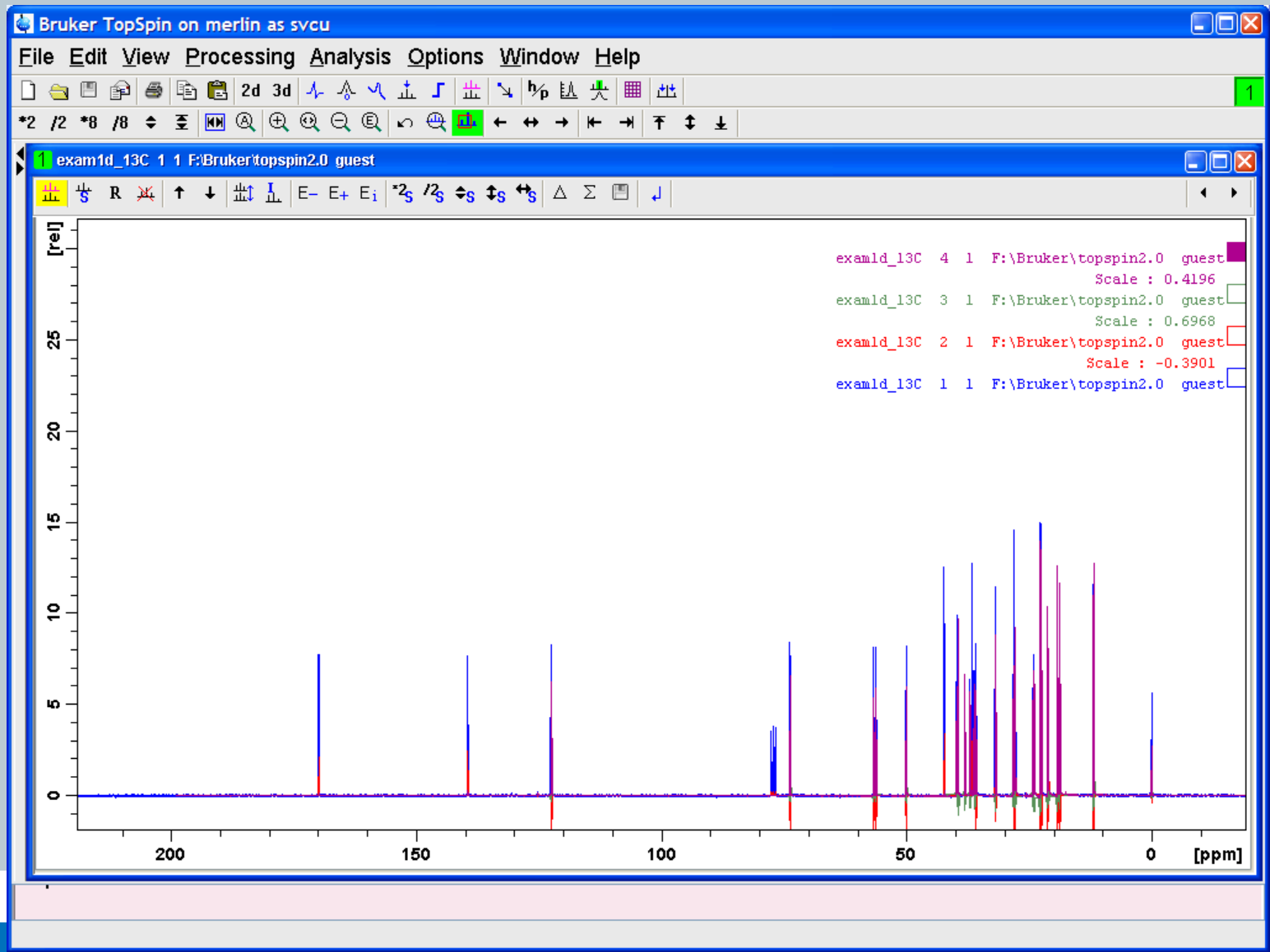
External editor

The preferred external editor as defined in Options → Preferences will always be used. For read-only files the internal editor will be taken.

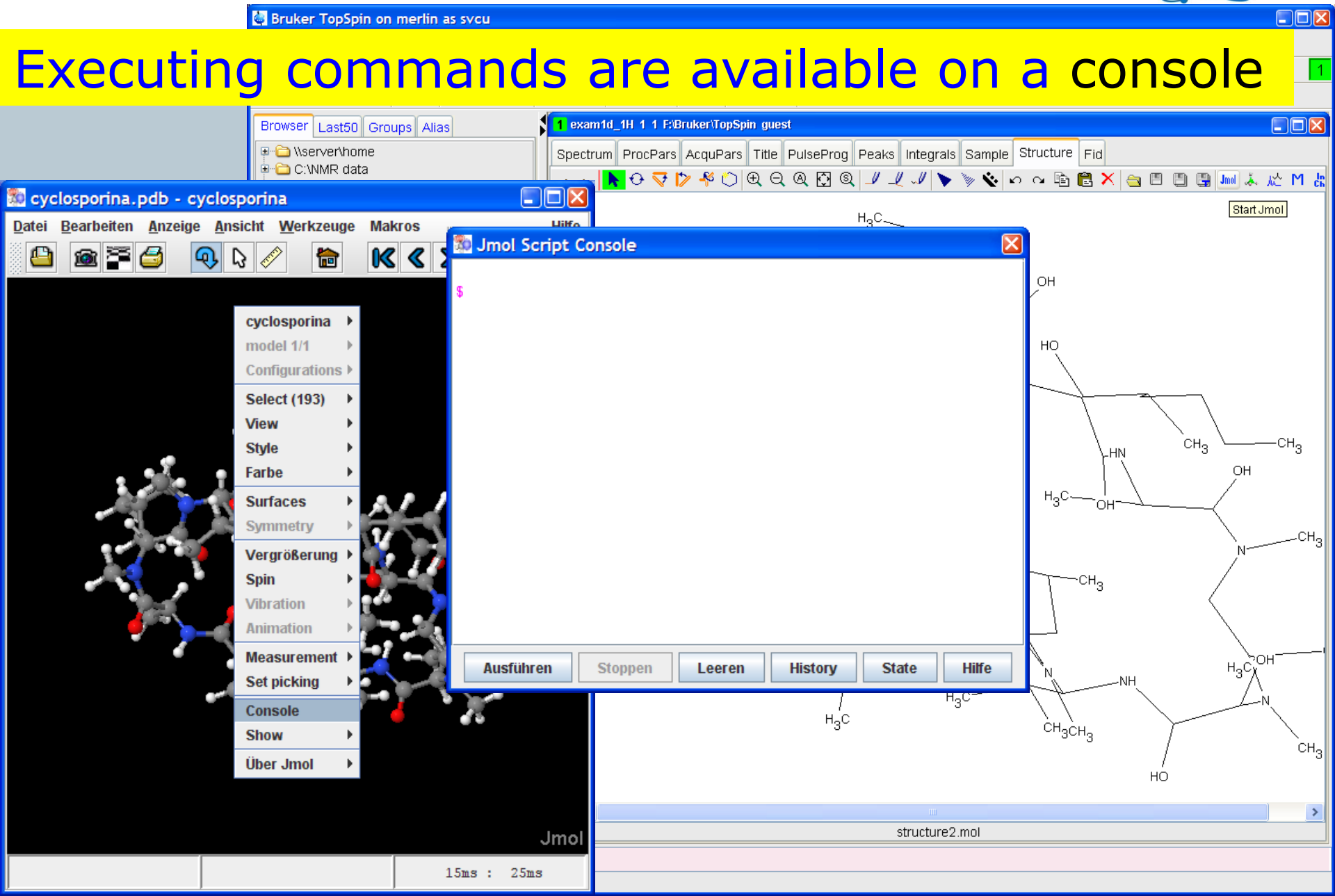


1D multiple display

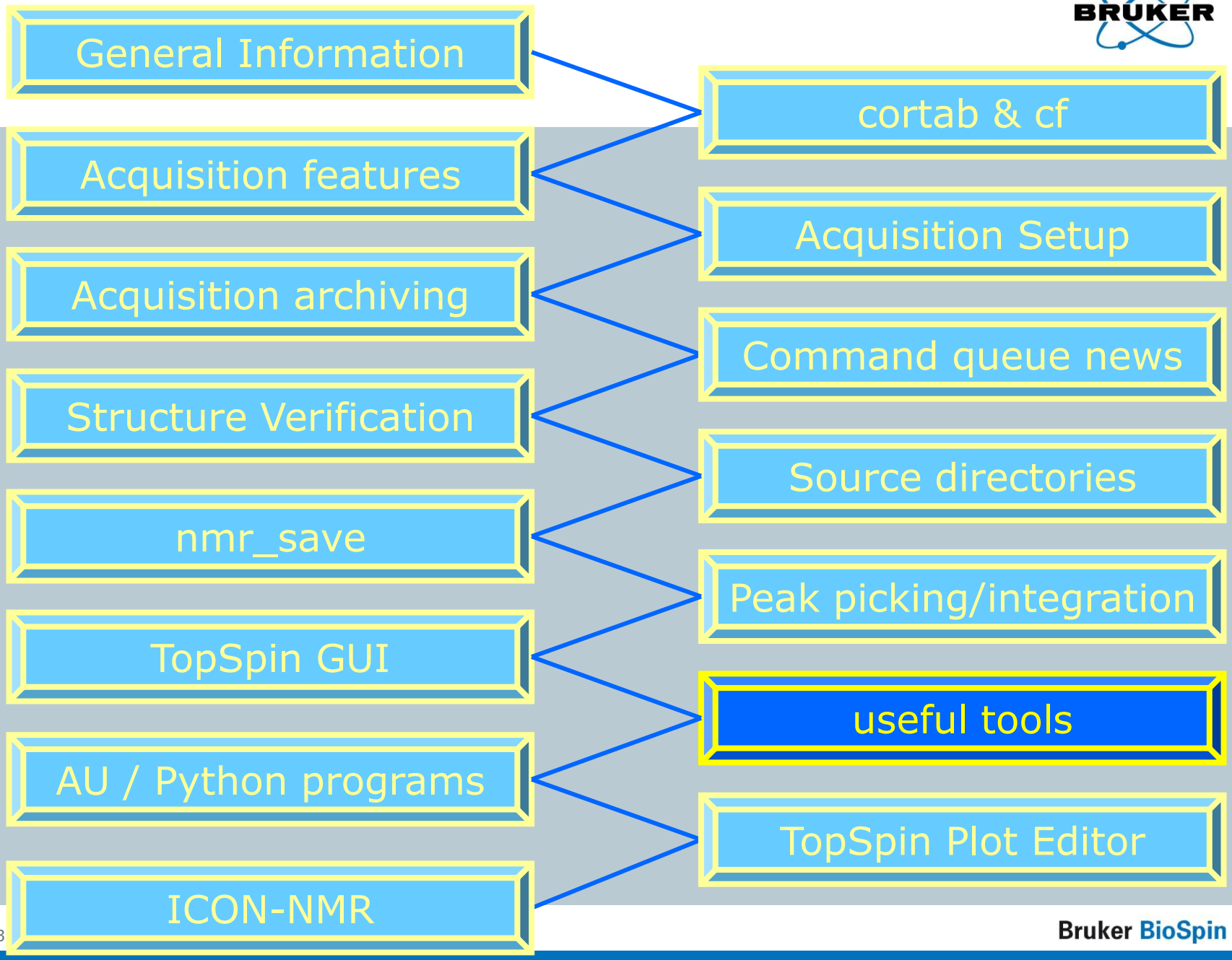
Dataset rectangles visible also with display on-top



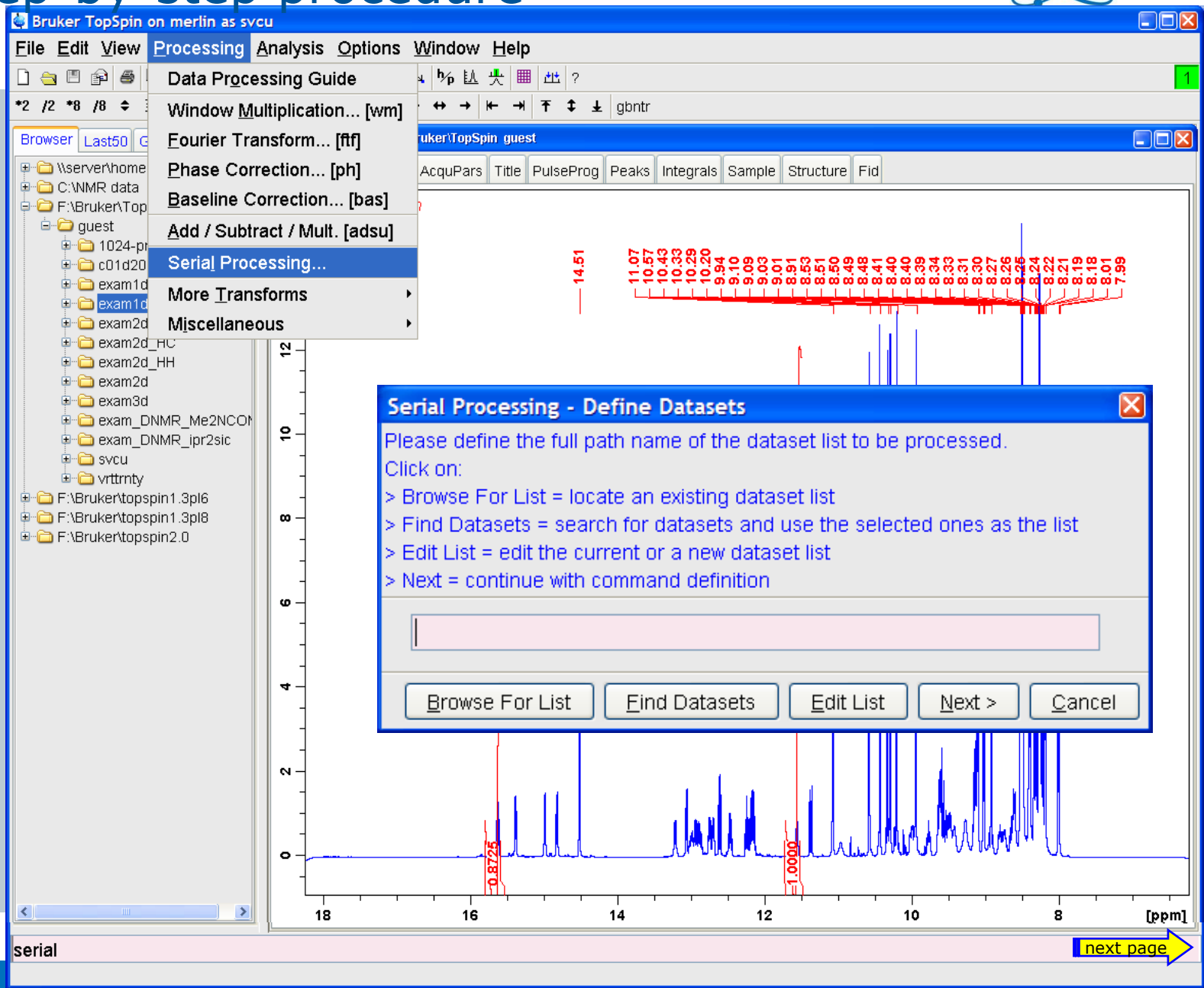
JMOL comes within a separate window



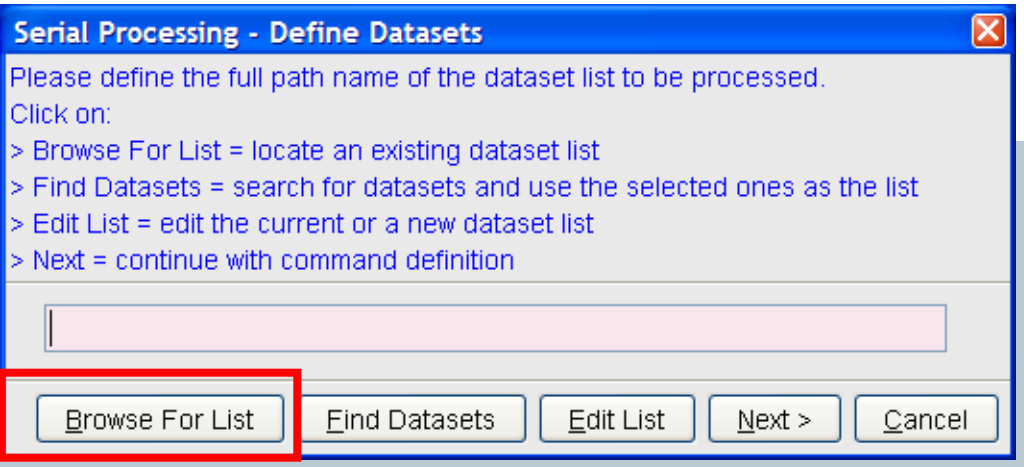
Content

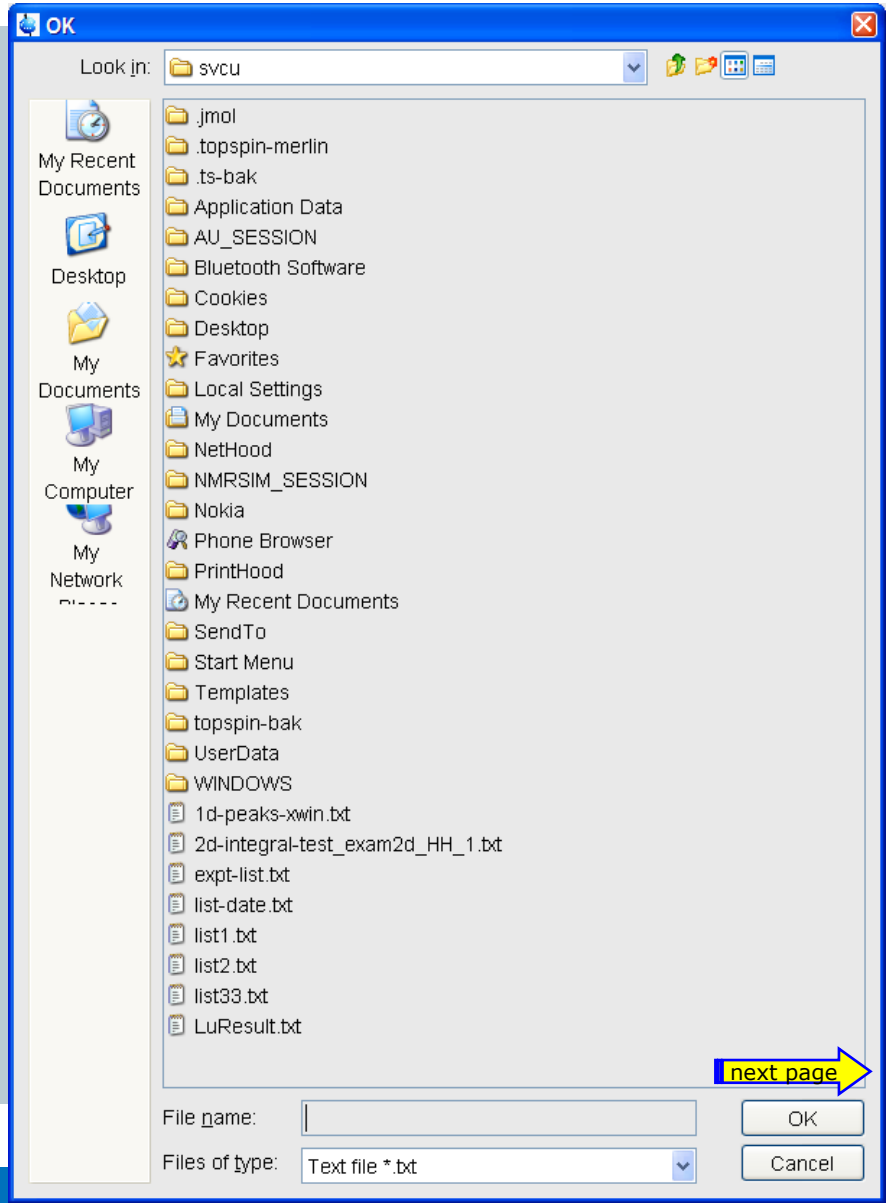

General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

Serial Processing –
revised step-by-step procedure

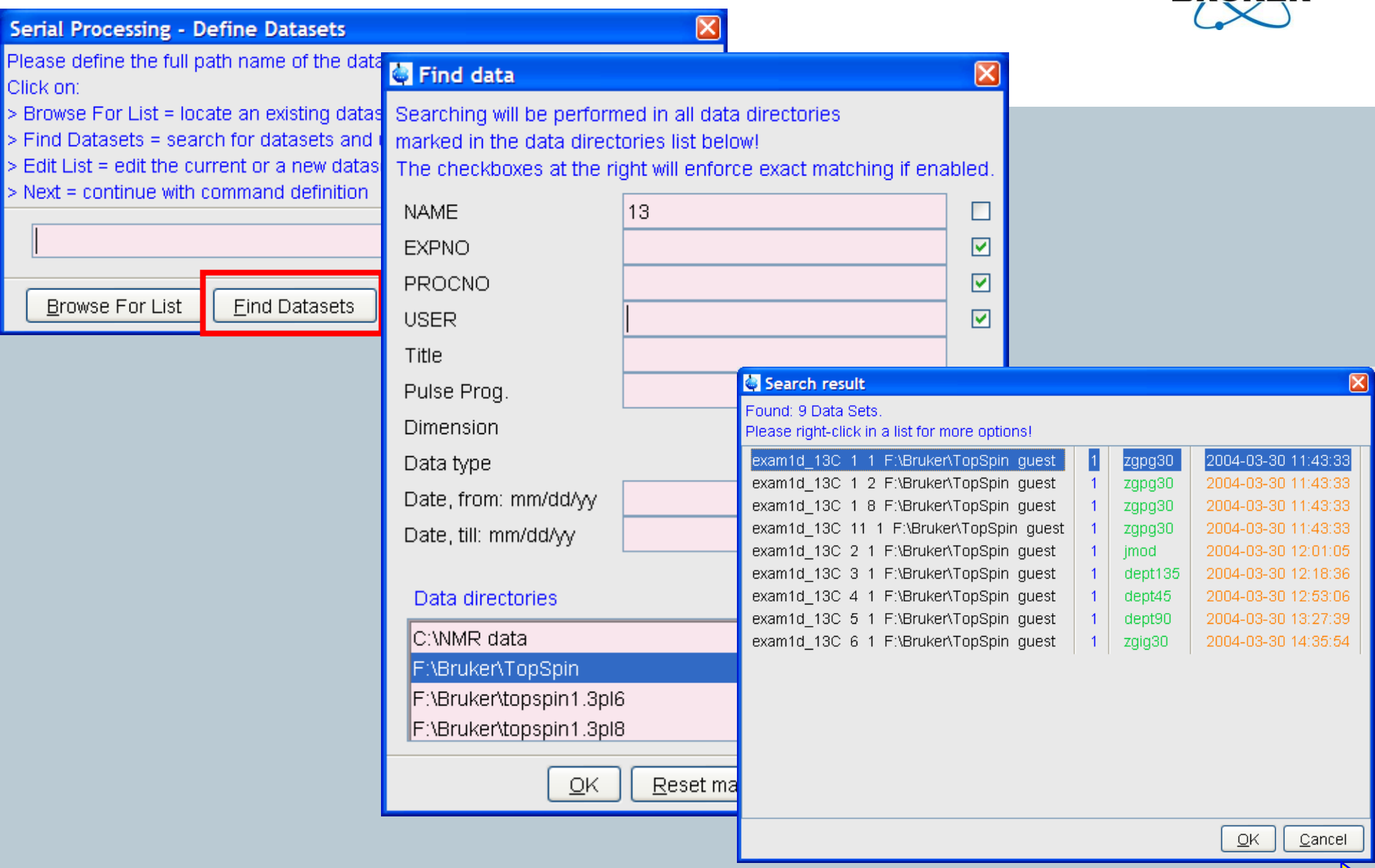


Serial Processing

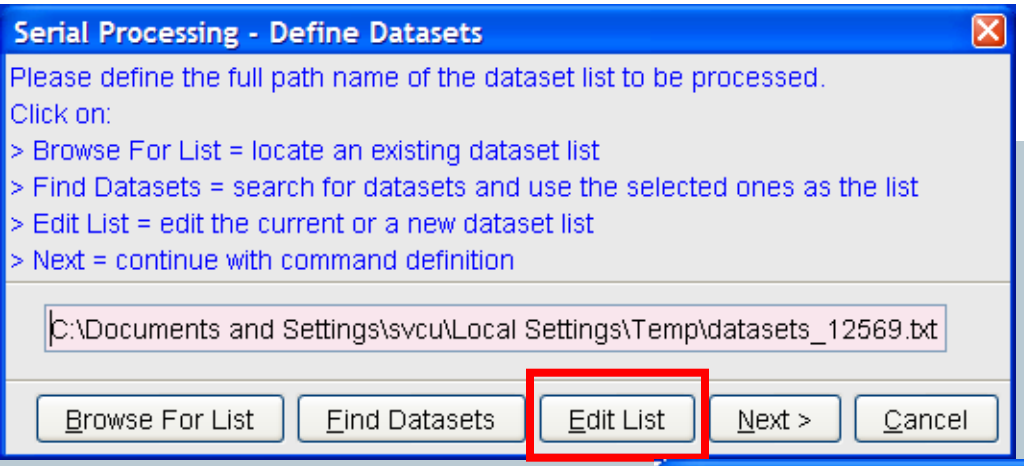


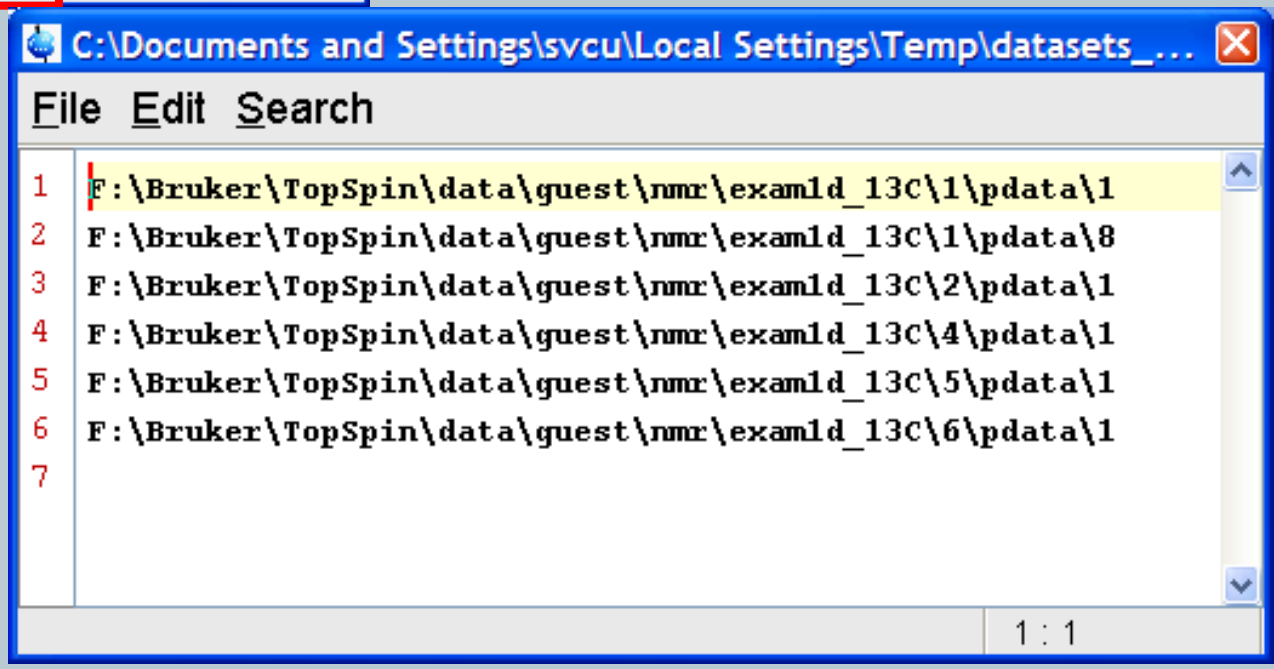


Serial Processing

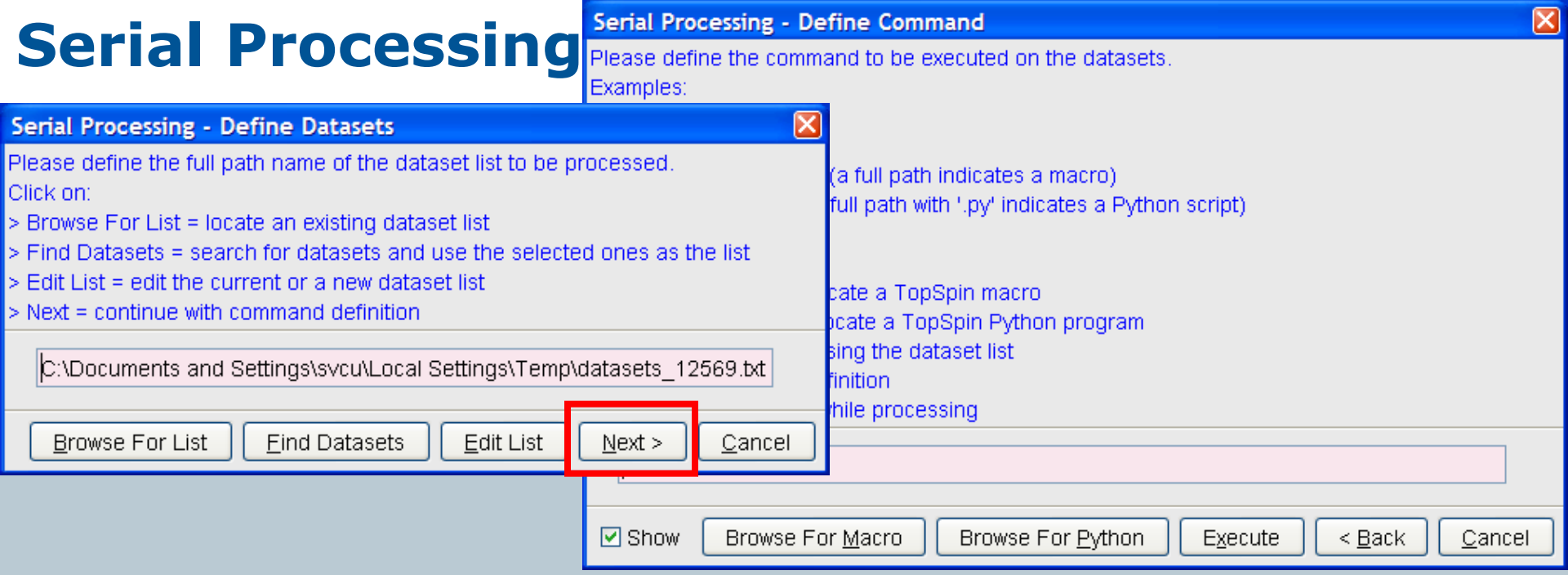


Serial Processing

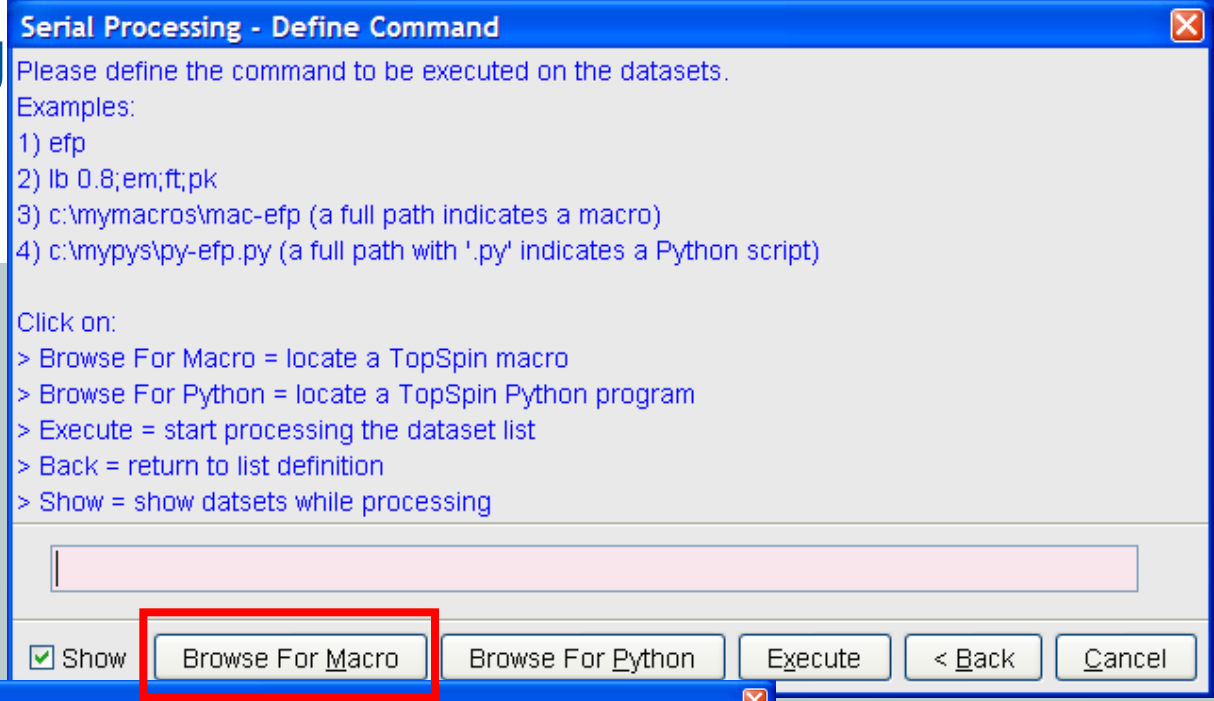


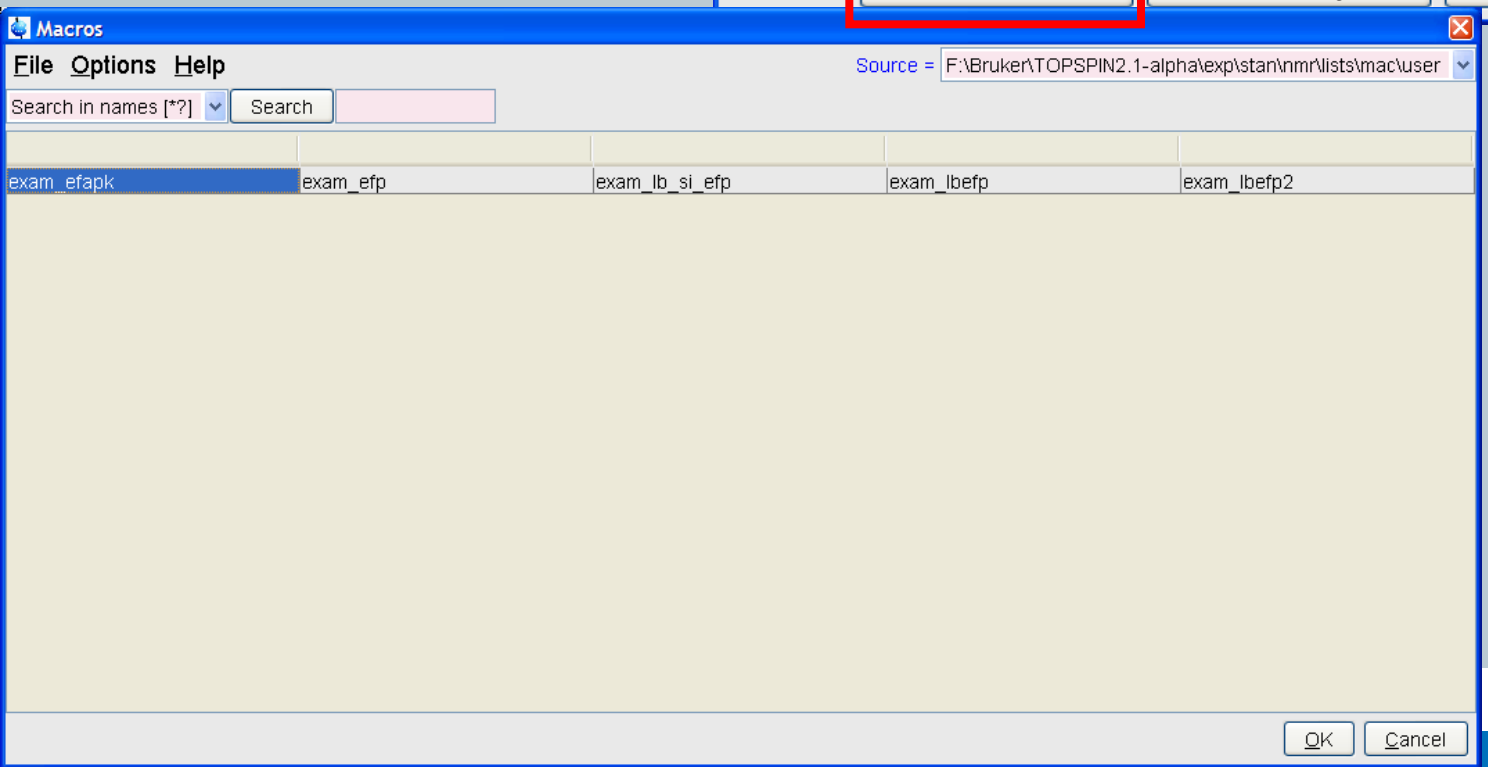


Serial Processing



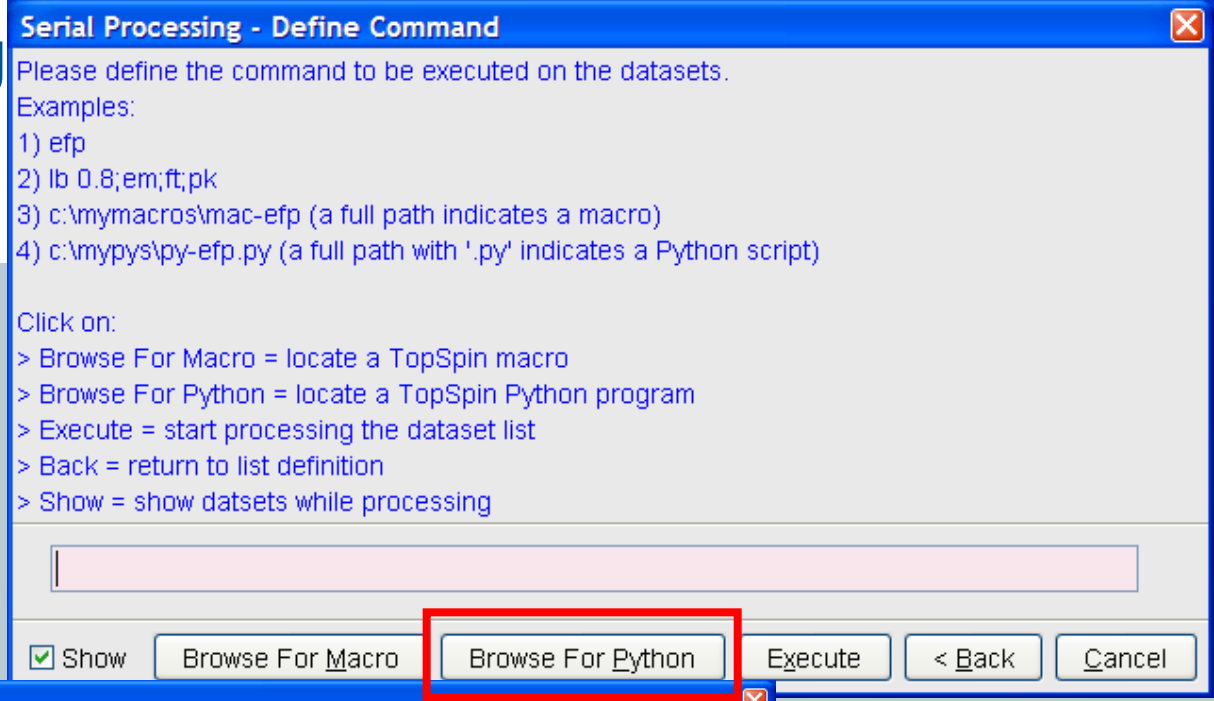
Serial Processing

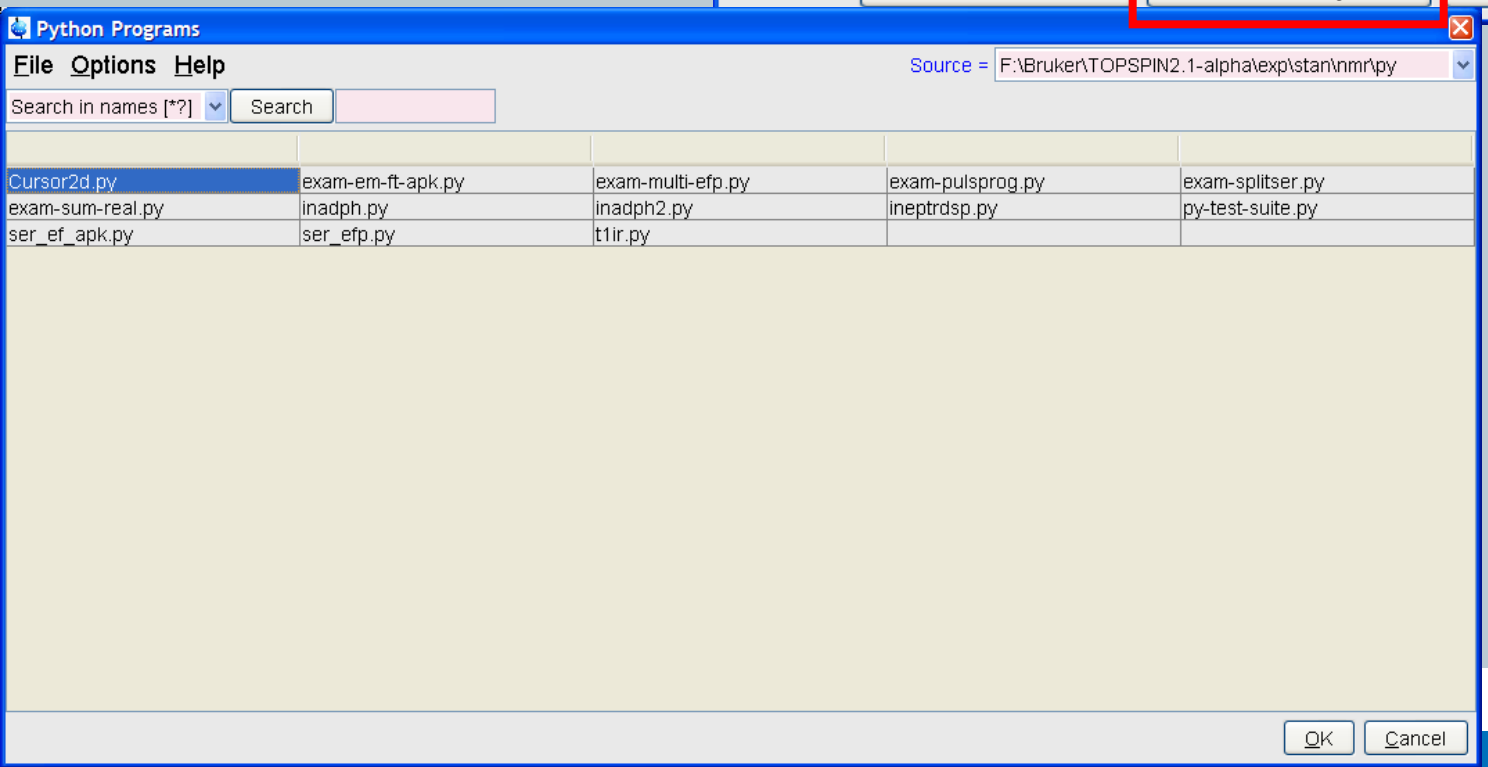




next page

Serial Processing

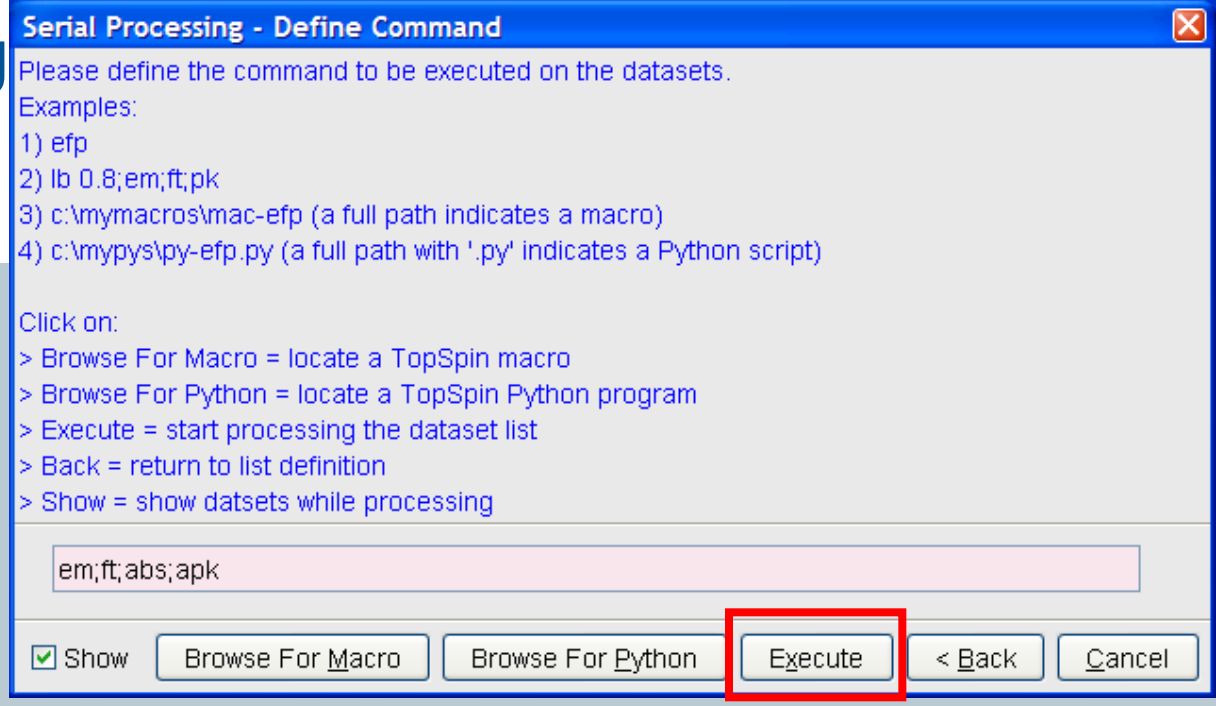


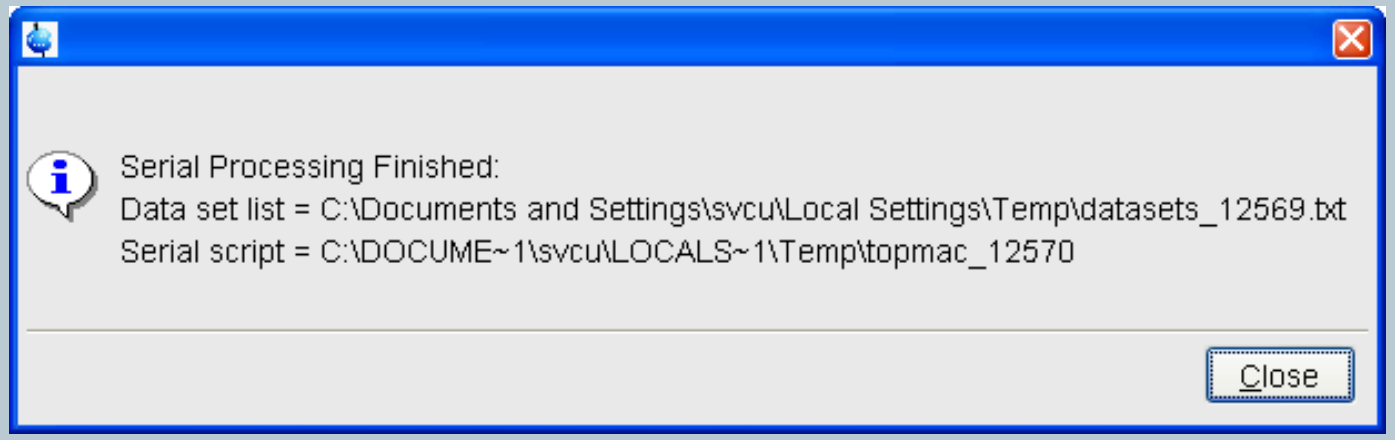


next page

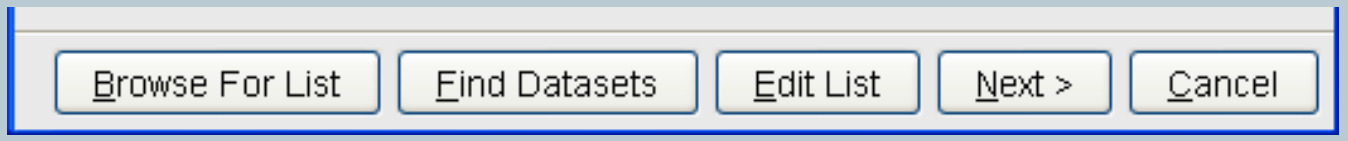
Bruker BioSpin

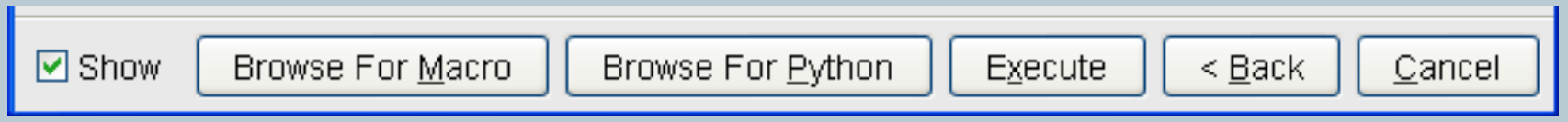
Serial Processing



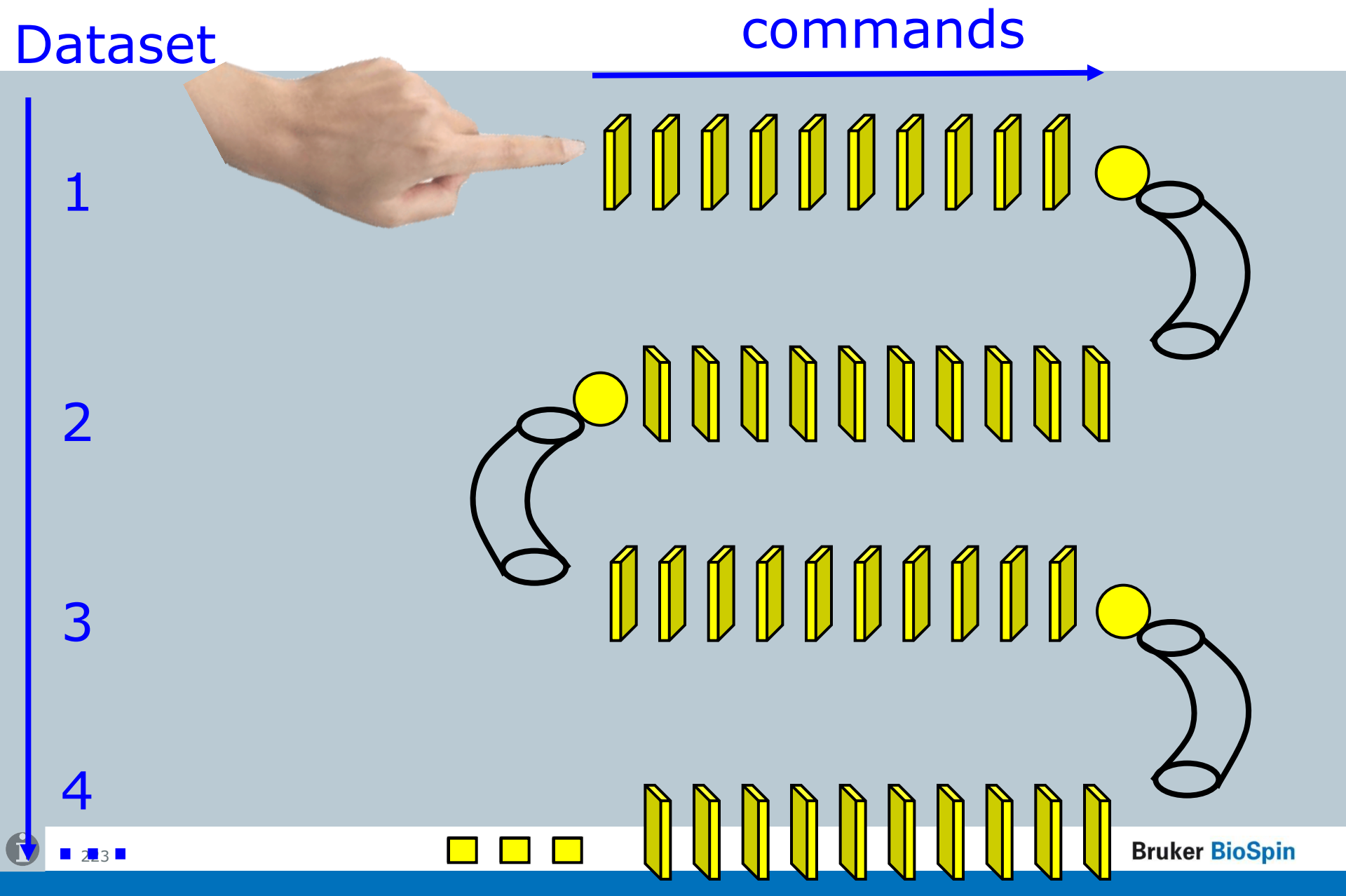


Serial Processing

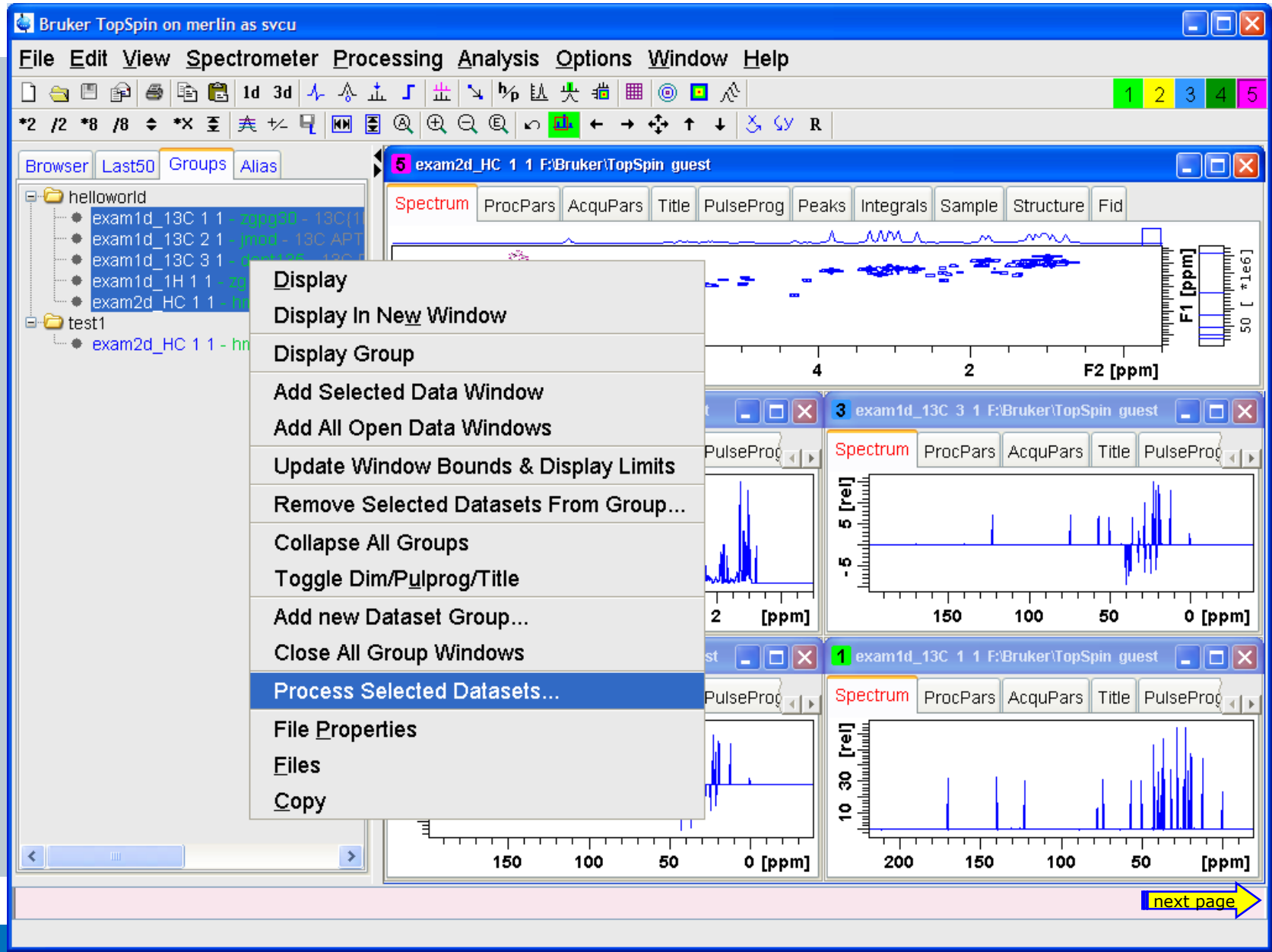




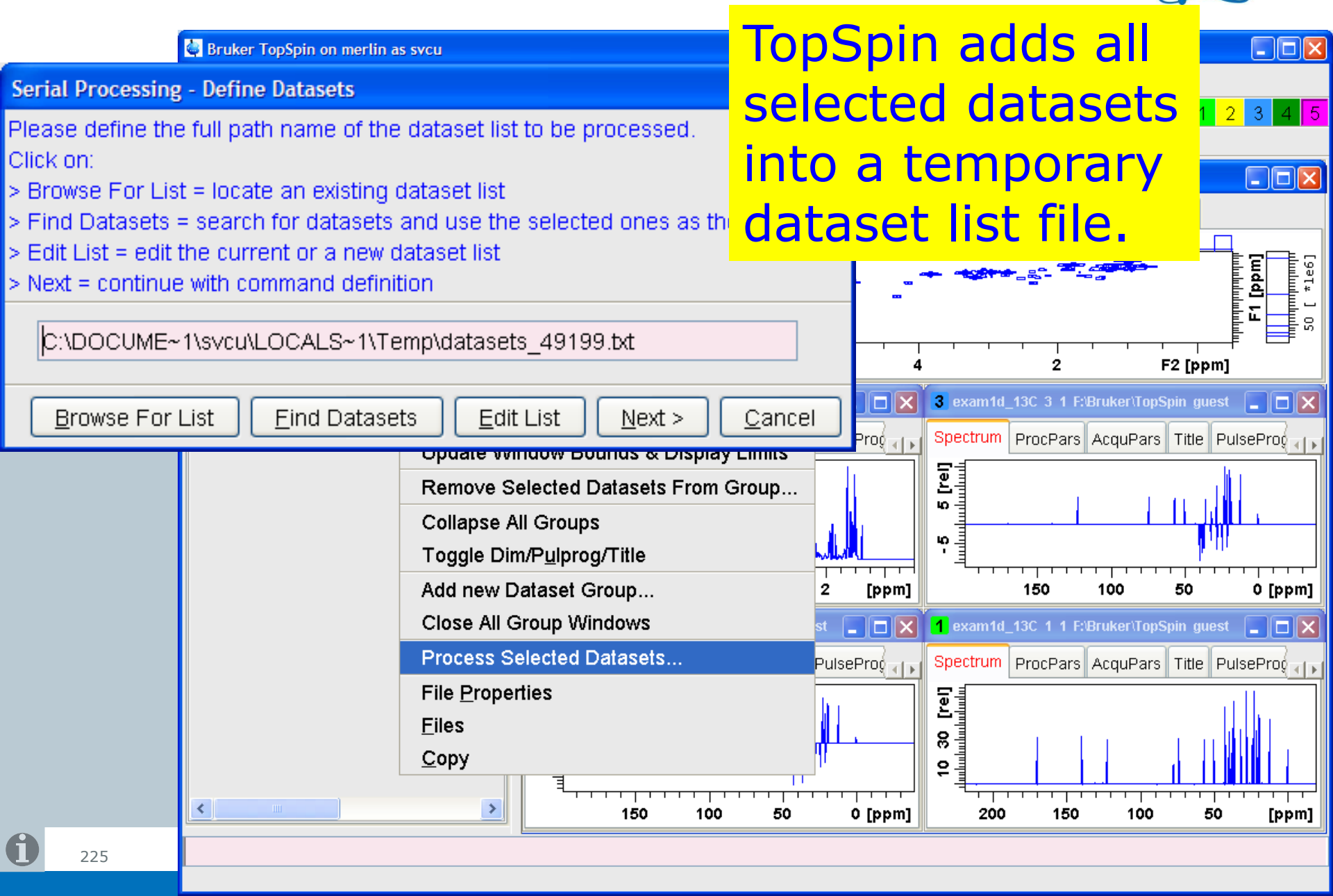
Serial Processing



Group members meet **serial processing**



Group members meets **serial processing**



New command – **nmrq**

The **nmrq** command is required to perform reliable quantitative analysis of 1D spectra comprising complex overlapping spectra. The program is able to:

- Perform mole ratio calculations given integral heights and number of protons per signal.
- Perform absolute weight calculations given the information detailed in plus molecular weights of all components and the weight of a reference component.
- Permit analysis of spectra characterised by poor baseline.

expl command with new options

- **expl spect**
  opens explorer window in:
  TOPHOME/conf/instr/<currently configure instrument>
- **expl prop**
  opens explorer window in:
  USERHOME/.topspin-<NAME_OF_PC>/prop
- **expl help**
  shows all available options (top, home …)

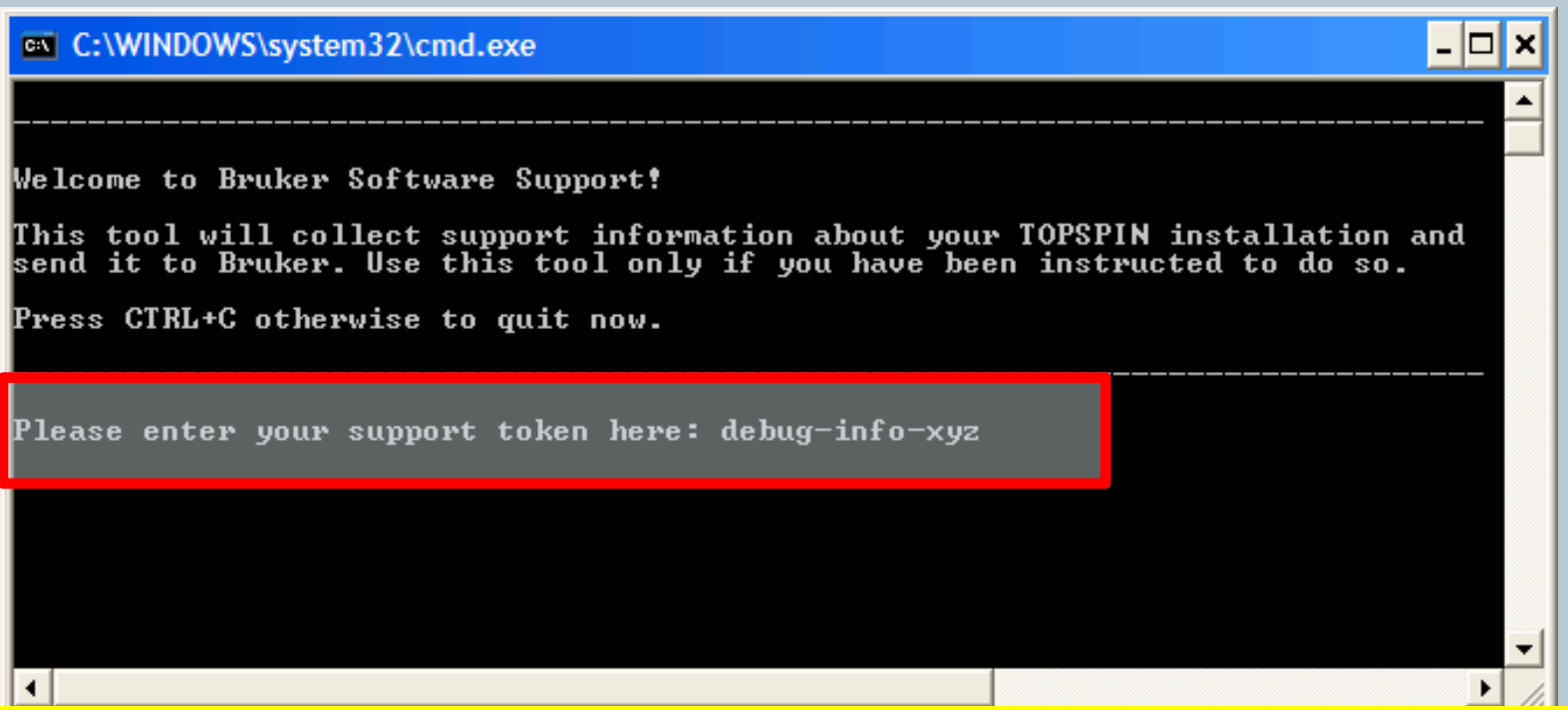
rpar behaviour has been improved

The command **rpar** will not delete existing data if there is no change of the dimension.
This allows e.g. reading in processing parameters for special processing purposes on existing data.

Script ‘savelogs’ goes online

The savelogs script has been improved.

If you are asked by Bruker to send debug information you can easily give the results file the dispatch number, the script will place it automatically on the Bruker FTP server.



next page

savelogs can be started under Windows from **Bruker Utilities** → **Miscellaneous** or under Linux just by typing the command in a shell

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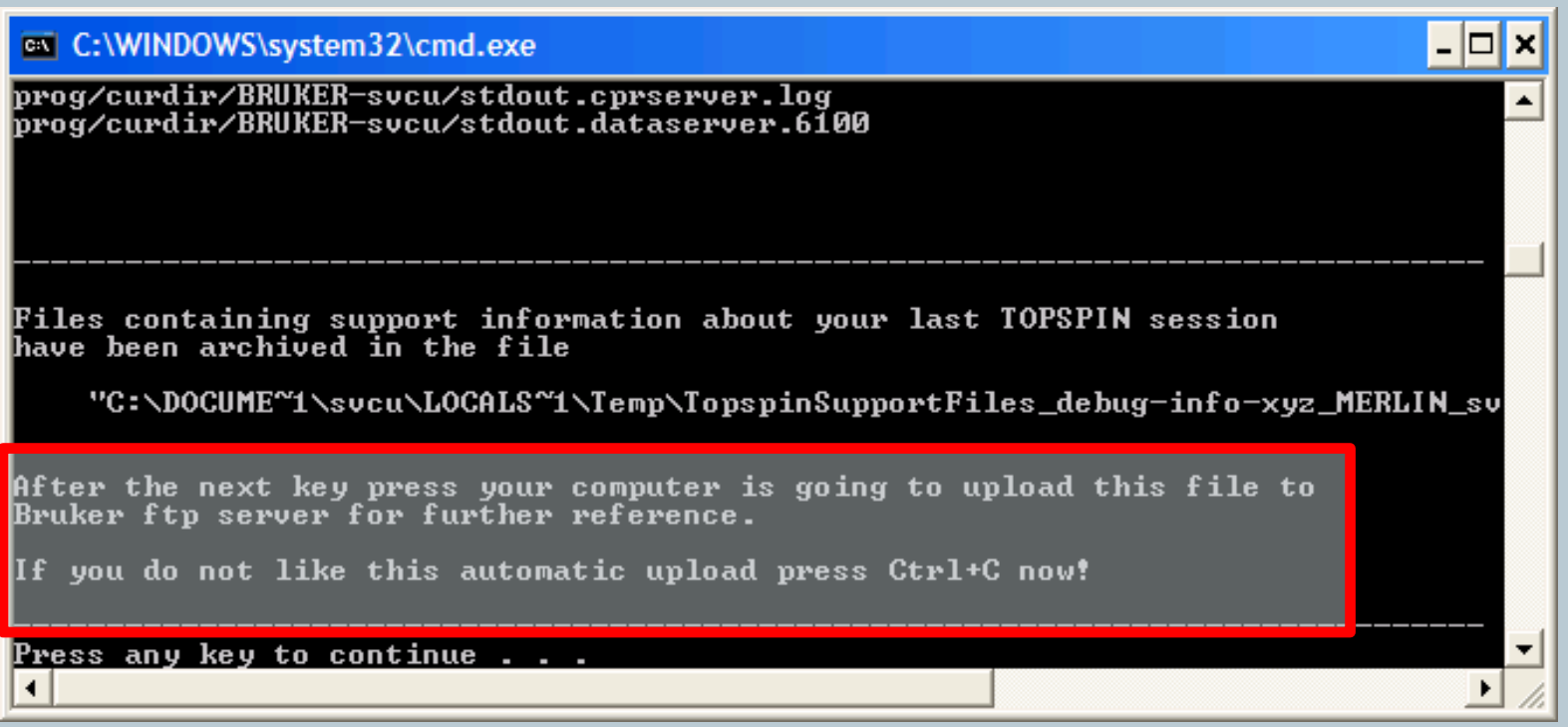

next page

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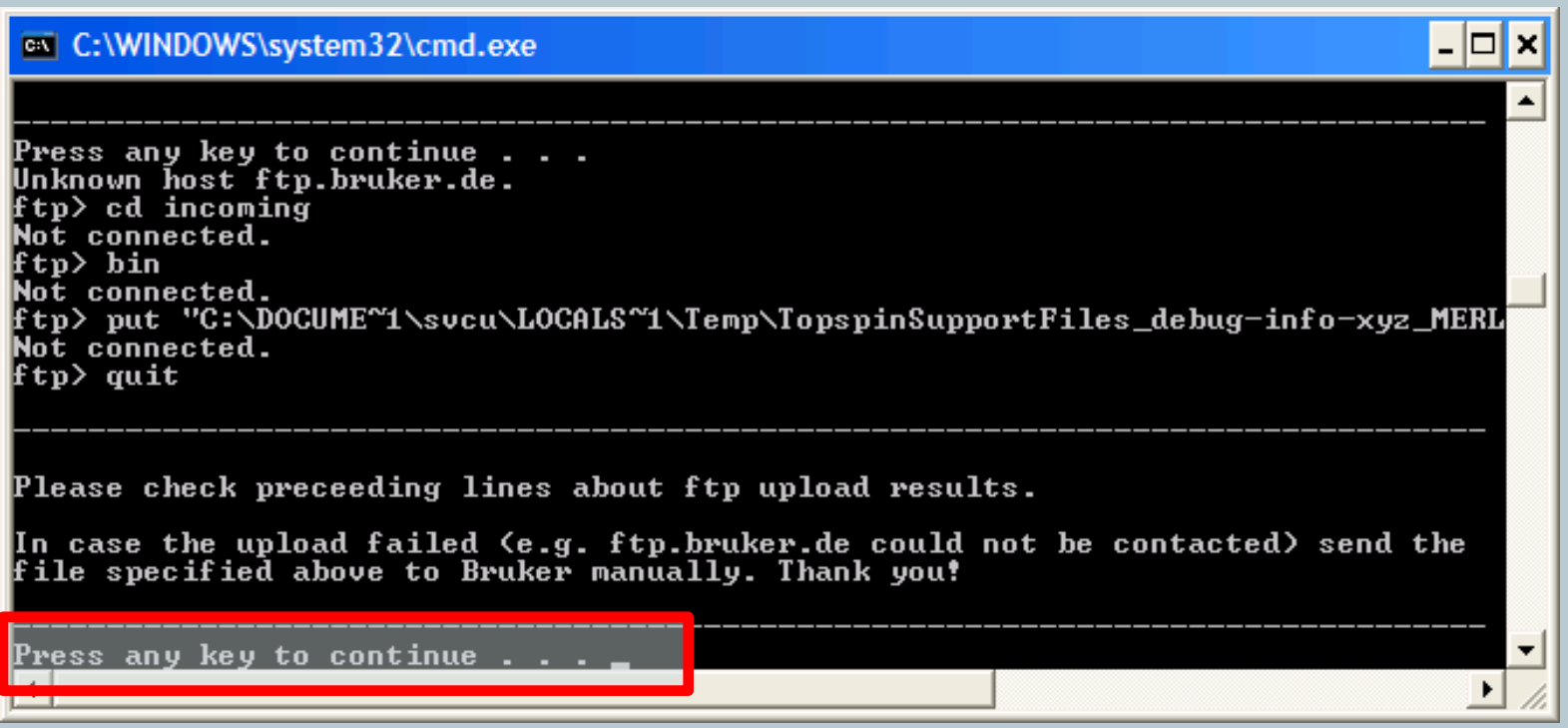
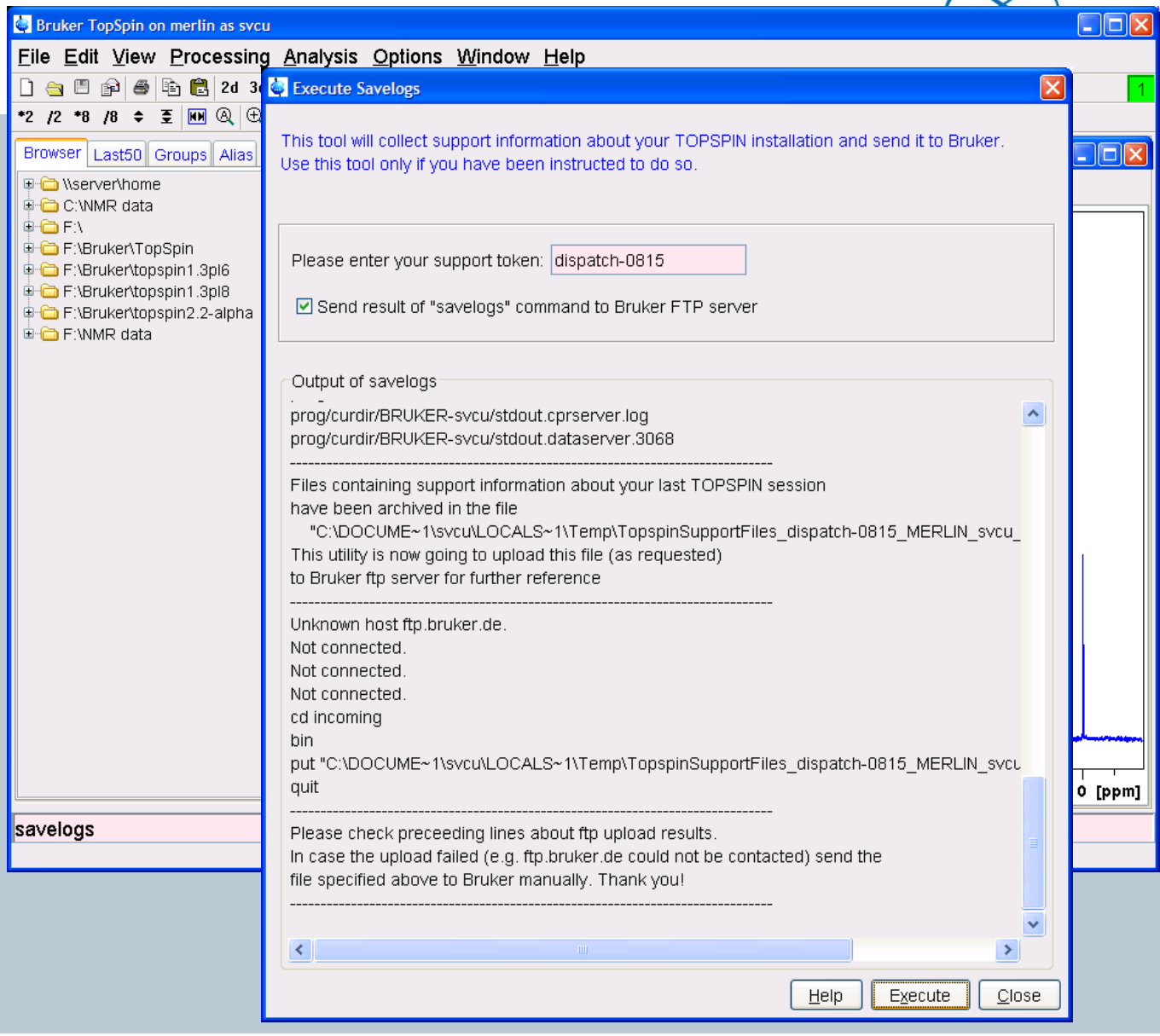


next page

savelogs can be started from within TopSpin

TopSpin offers the new command **savelogs** which calls internally the script savelogs



New feature for backbone assignment

TopSpin includes the AutoLink backbone assignment algorithm.

This software analyses the peak information available on a given set of protein spectra and calculates a backbone assignment.

next page

New command - autolink

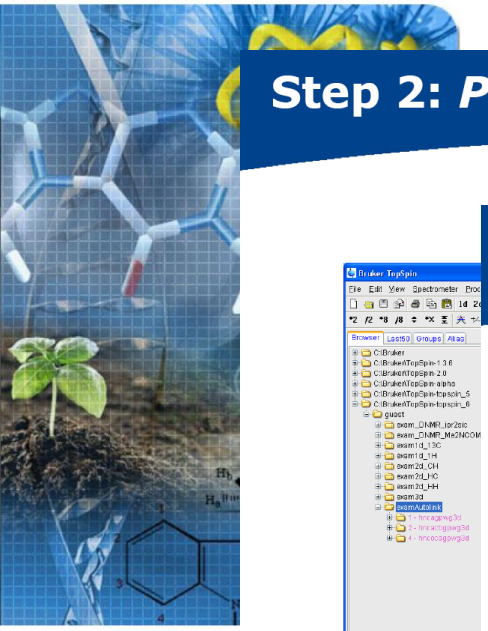
Syntax: **autolink** or

Analysis → Proteins → Automatic Backbone Assignment

The Help button in the AutoLink window opens a manual which guides you step-by-step through the setup of an Automatic Backbone Assignment.
The molecule Ribonuclease-T1 is used as an example in this manual.
The respective datasets are available with the example datasets of TopSpin 2.1.

next page

AutoLink Tutorial



Step 2: *Process data*

Fig. 2: Process e

Step 6: *Review results*

The assignment view is organised in a tree, where the outer level contains the residue sequence.

Expanding any re

calculated assign

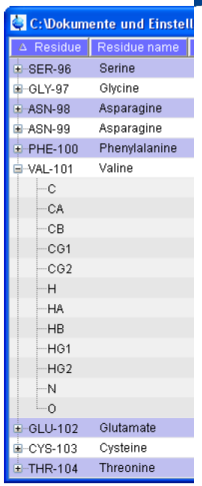


Fig. 10: The ass
displays the calcu

Step 6: *Review results*

Once the software has create peak annotations based on the calculated assignments, the results may immediately be reviewed on the *Peaks* tabulator in the respective dataset windows. The generated information includes the assignment of each frequency component for a given peak.

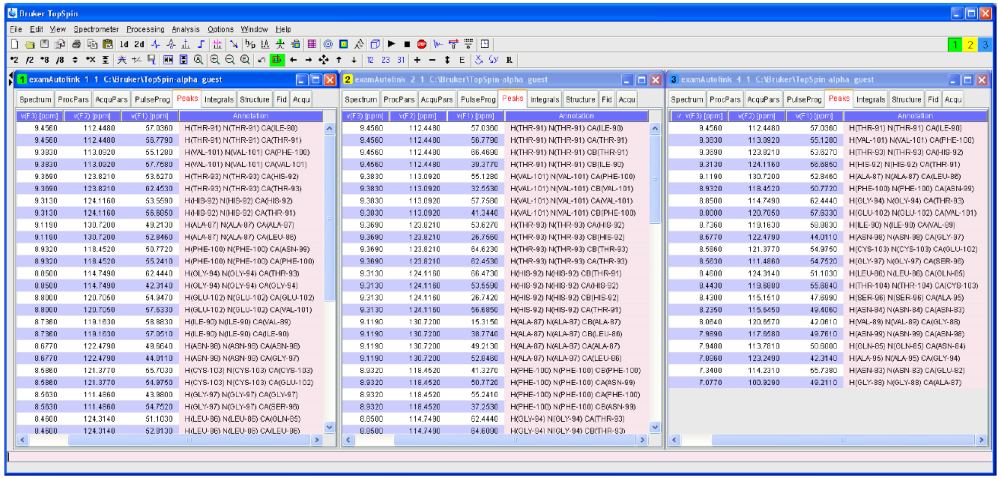


Fig. 12: The annotated peak lists of *Ribonuclease-T1*. The annotations are generated based on the assignments calculated by AutoLink.

New command - **auremol**

Syntax: **auremol** or

Analysis → Proteins → Auremol

The Protein Structure Elucidation Tool AUREMOL can now be started easily from within TopSpin.

Auremol requires a separate license, but each new Full und Processing_only TopSpin license offers automatically a 6-months demo license for Auremol.
A separate demo license can be ordered anytime under: www.bruker-biospin.com

next page

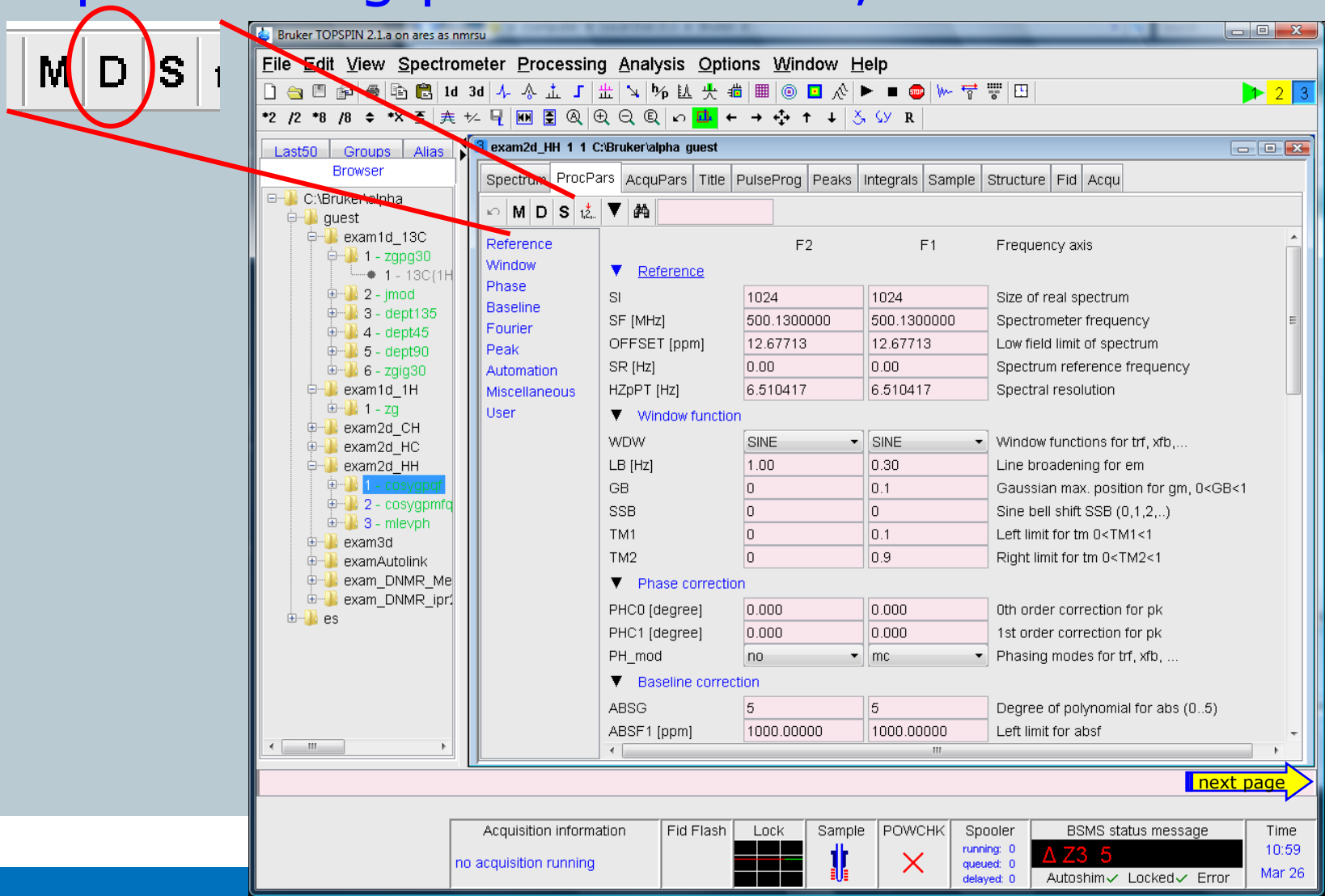
Auremol filter for peak tables

AUREMOL master list files can now be easily im- or exported from within the TopSpin peak list.

DOSY parameter

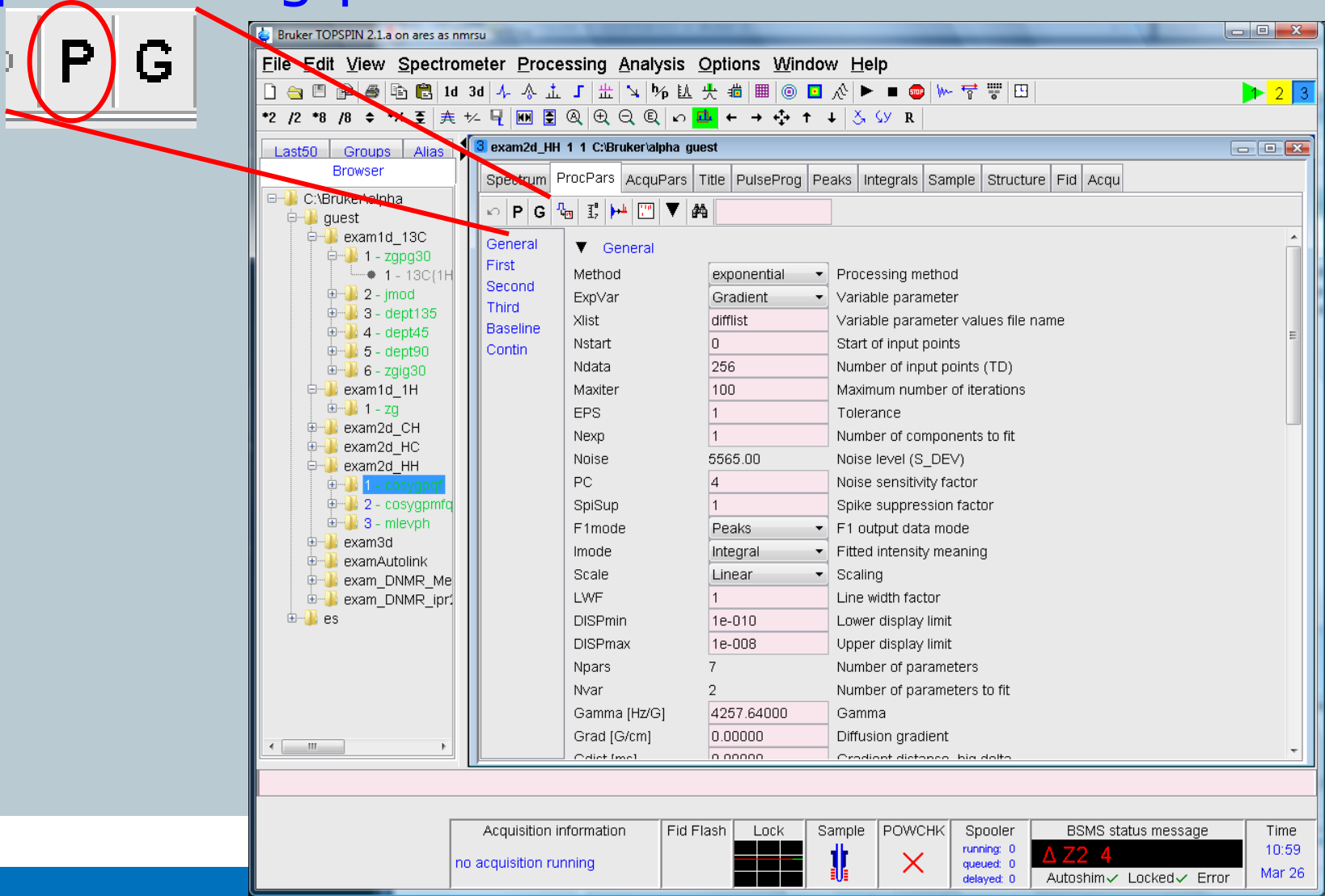
DOSY parameters are accessible after **eddosy**

from the processing parameter tab, click on: D



DOSY parameter

To jump back from the DOSY parameter list to the processing parameters click: P



MAXENT is back

MAXENT (maximum entropy), the alternative for deconvolution is available in TopSpin 2.1.

MAXENT requires a separate license.
A demo license can be ordered anytime under: www.bruker-biospin.com

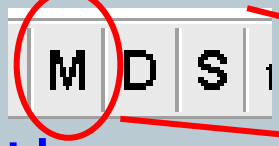
next page

MAXENT is back

Parameter for MAXENT (maximum entropy)

are available from the Processing Parameters Tab,

click on: M



or use the command:

edmax

New format for Export: PDF

Export of what is shown in the current dataset can now be stored in PDF format.

Furthermore it can be executed directly from TopSpin command line:

exportfile <path>/<filename>.pdf

Zipfile from command line

The command **tozip** can be executed on the command line with all arguments:

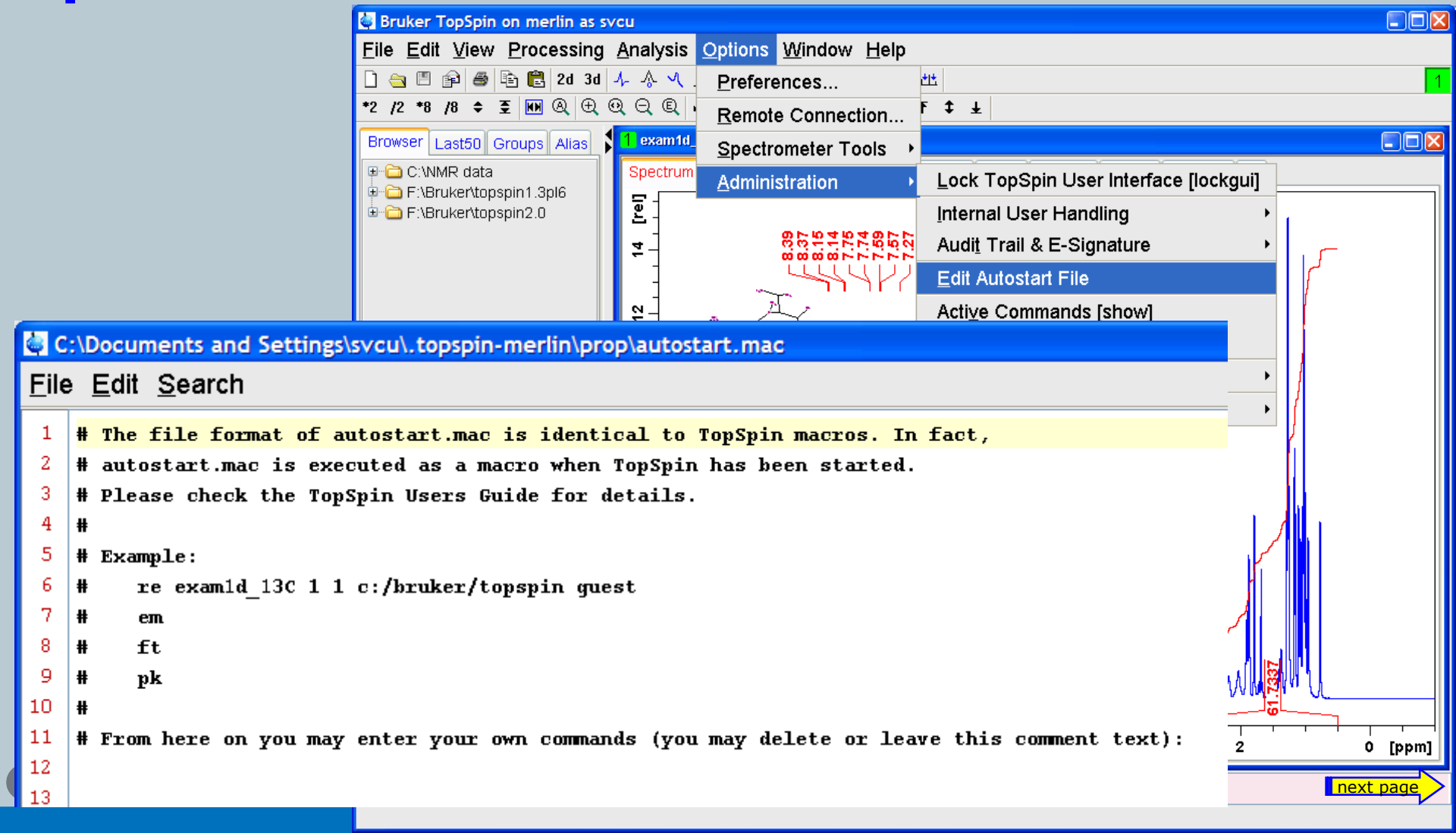
tozip –d <path>/<filename>.zip

If the graphical user interface should be used, simply use the command **tozip**

Autostart

Autostart actions can be configured from the menu:

Options → Administration → Edit Autostart File



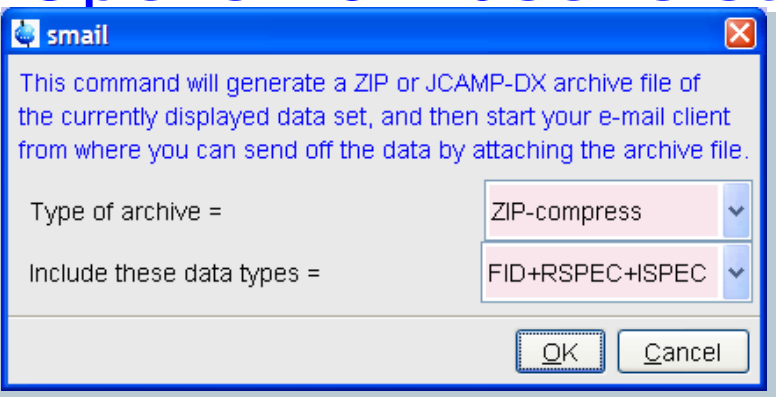
Autostart used already in previous TopSpin versions?

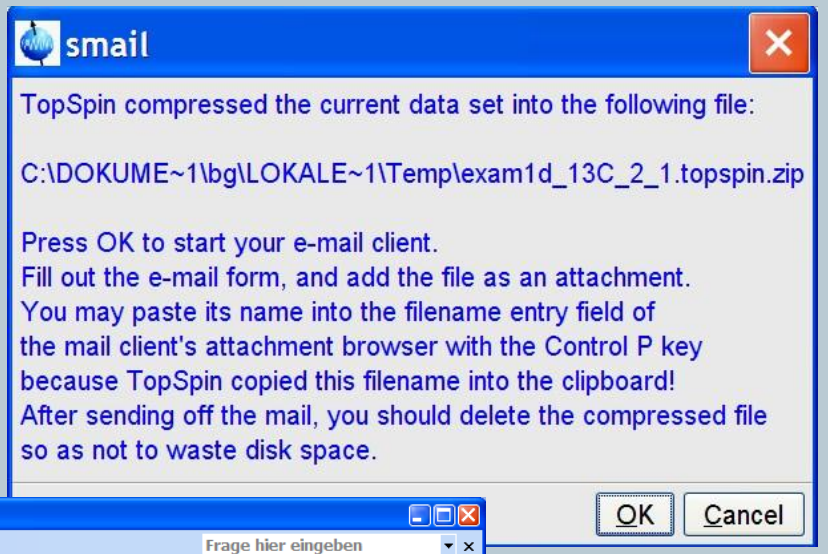
The syntax of the autostart-file has been improved. It is now possible to enter simply any TOPSPIN command that should be executed, one per line.

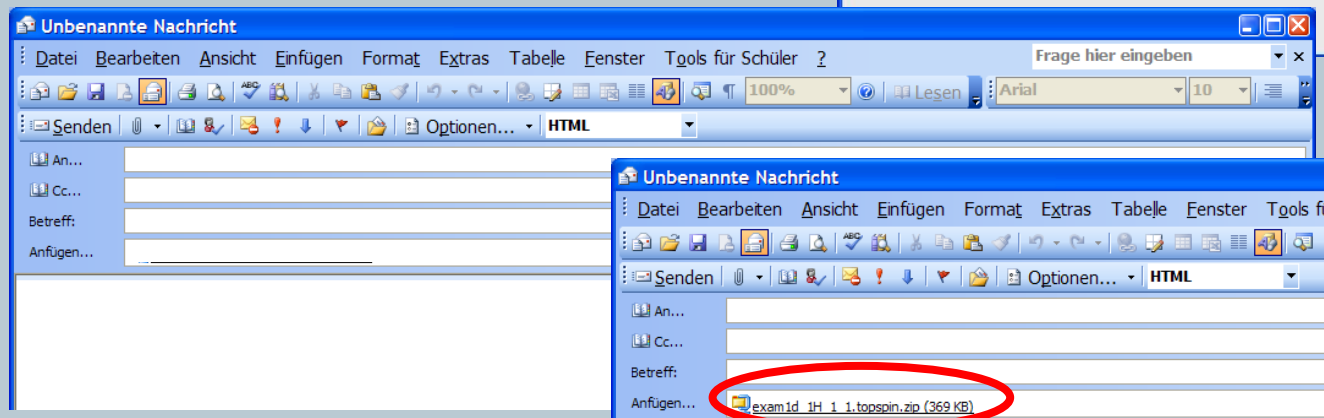
If an autostart-file of a previous TOPSPIN version is available it will be read with the first start of TOPSPIN 2.1 and the content will be saved in the new format.
From now on only the new file will be used for TopSpin 2.1.

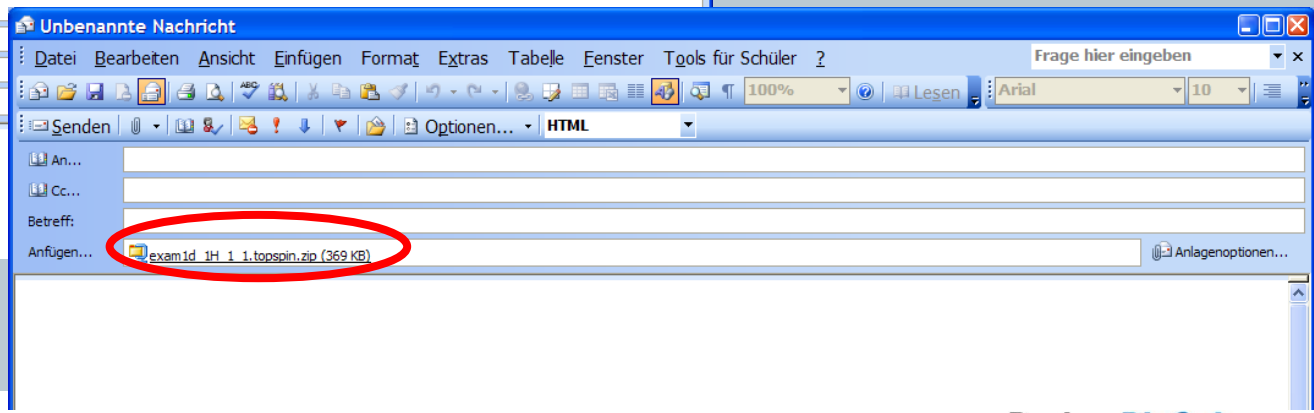
Command **smail**

Opens now user's standard email client









Restarting the GUI which has been started by CPR

restartgui

Windows: Bruker Utilities → Miscellaneous

Linux: Shell

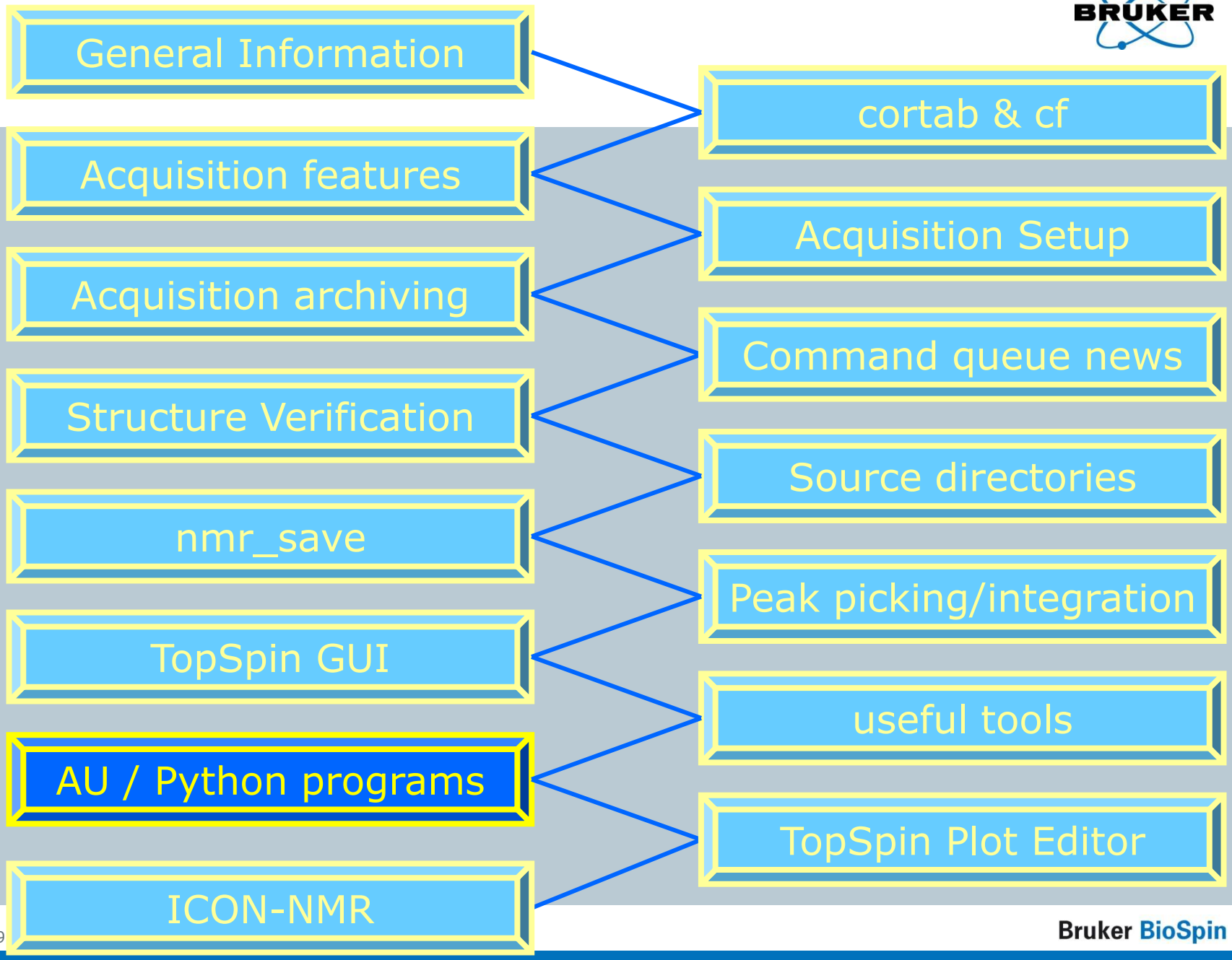
To restart the CPR-GUI from a second window / remote connection, use TopSpin command:

restart

Installation

TopSpin can now be installed on directories mounted via NFS.

Content


General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

New Python manual

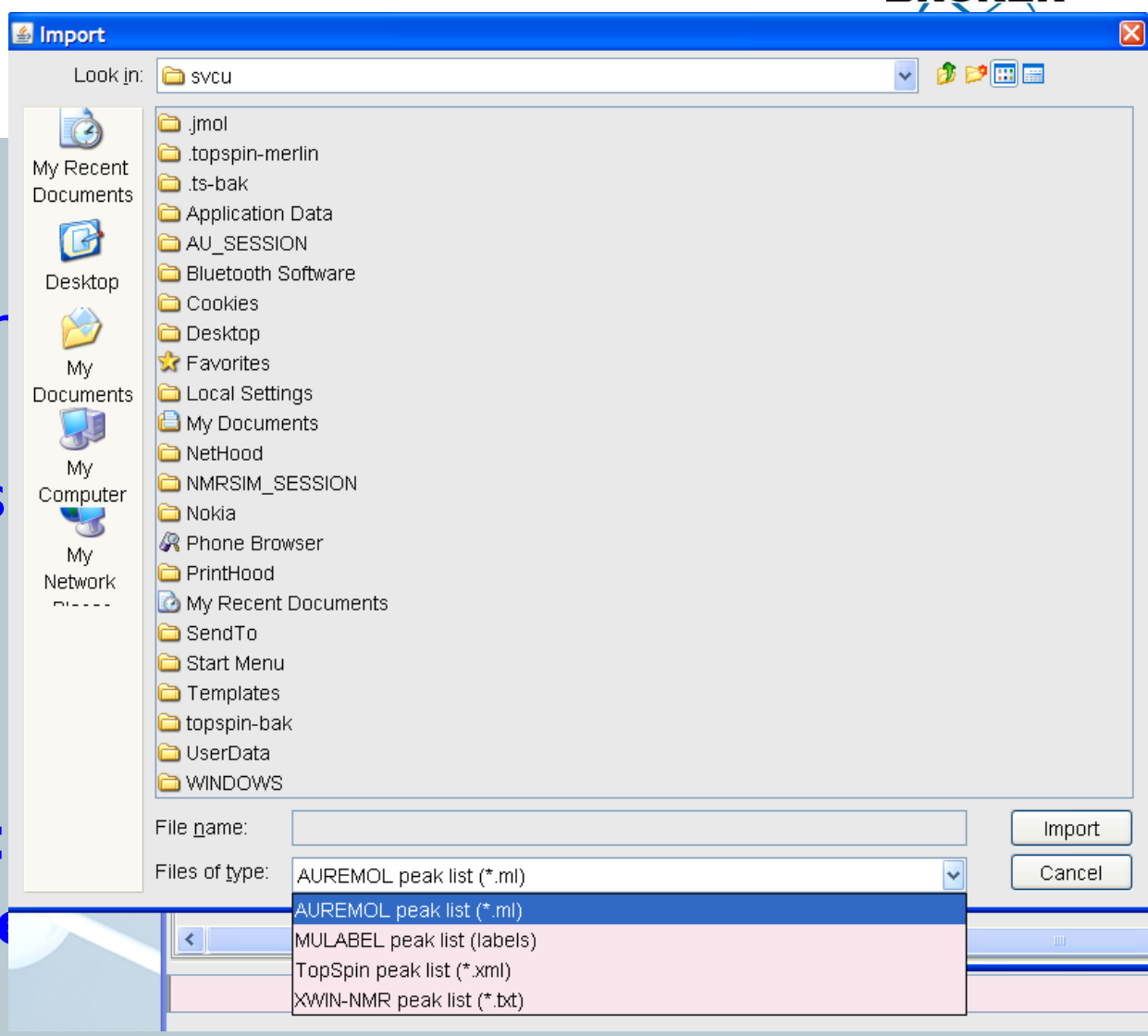
Introduction into python:

New 60-page overview manual.

AU program: mulabel

Import command for ‘labels’ file as annotation for peaks

- Right mouse click in peak table
- TopSpin command: **peakstransferlab**



With option to overwrite existing annotations and/or value delta for differences in peak shifts

New handling of AU program macro '**XAU**'

The AU program macro **XAU** is used to start a second AU program from an already running AU program.

The syntax of the **XAU** has been changed. In previous version it has been used like this:

XAU("<Name_of_AU_PROGRAM>");

In TopSpin 2.1 the new syntax is:

XAU("<Name_of_AU_PROGRAM>", "<argument>");

Note: Any AU program in TopSpin 2.1 that contains the **XAU** macro must be modified otherwise the compilation of the AU program will fail. All Bruker AU programs have been modified, but user-specific AU programs have to be modified by the customer.

For more details check the Release Letter of TopSpin 2.1.

New AU program macros

DELETEPROCDATA(name1,expno1,procno1,disk1,user1)

DELETEIMAGINARYDATA(name1,expno1,procno1,disk1,user1)

DELETERAWDATA(name1,expno1,disk1,user1)

DELETEPROCNO(name1,expno1,procno1,disk1,user1)

DELETEEXPNO(name1,expno1,disk1,user1)

DELETENAME(name1,disk1,user1)

New AU program macros

getParamDirs()

getParfileDirforRead()

getParfileDirforWrite()

For getting the information in AU programs about location of parameter files (pp, mac, AU …).

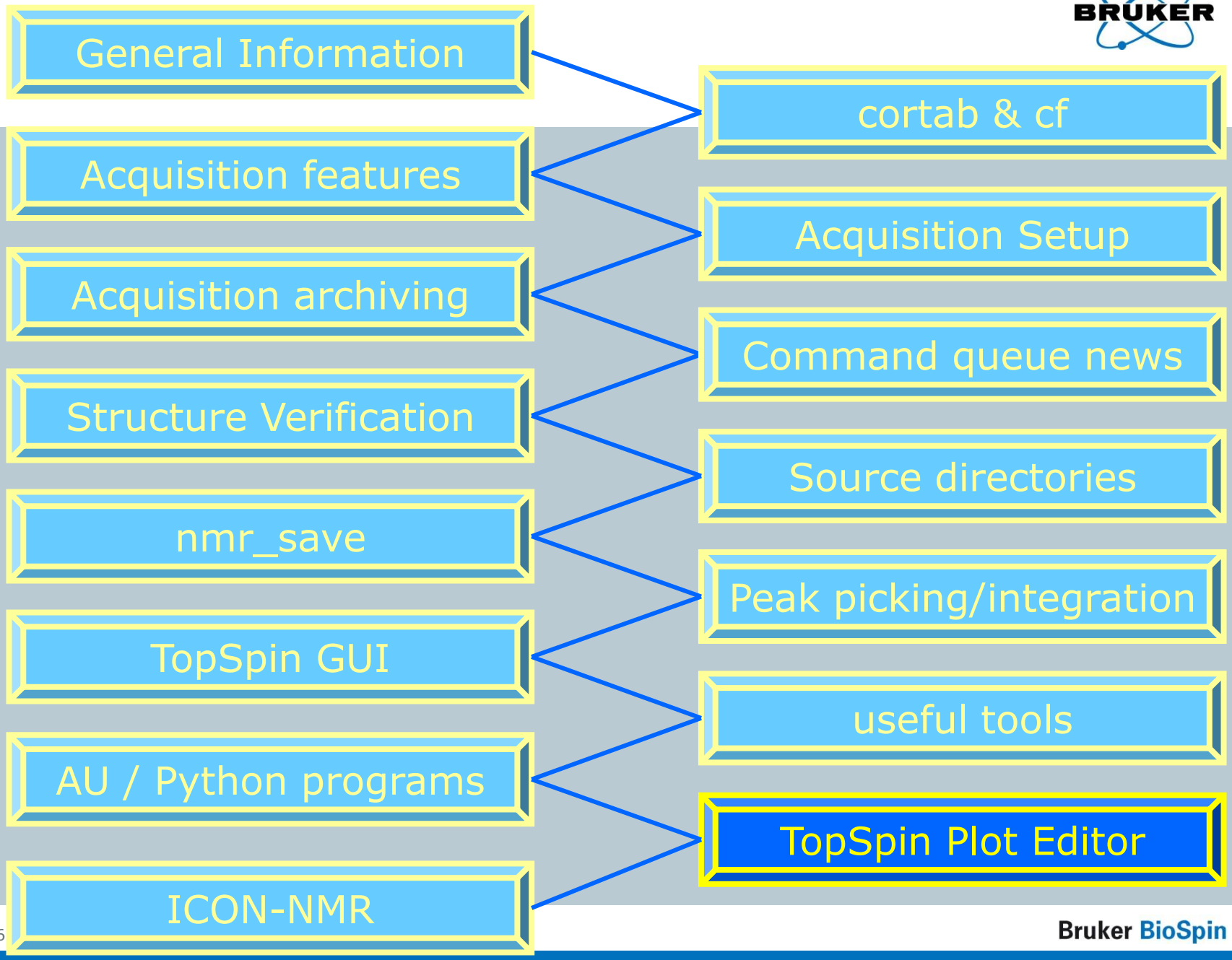
For more details check the Release Letter of TopSpin 2.1.

New AU program macros

TopSpin 2.0 and previous versions offered different functions to get path information of specific files, e.g.:
getstan which offered the path '*<TopSpin_Home>/exp/stan/nmr/*'
and
PathXWinNMRExpStan which offered the path
'*<TopSpin_Home>/exp/stan*'
Because with TopSpin 2.1 each user can store these files in any directory it is recommended to use the new AU functions:
getParamDirs(<keys>)
getParfileDirForRead(<name>,<key>,<var>);
getParfileDirForWrite(<name>,<key>,<var>);

For more details check the
Release Letter of TopSpin 2.1.

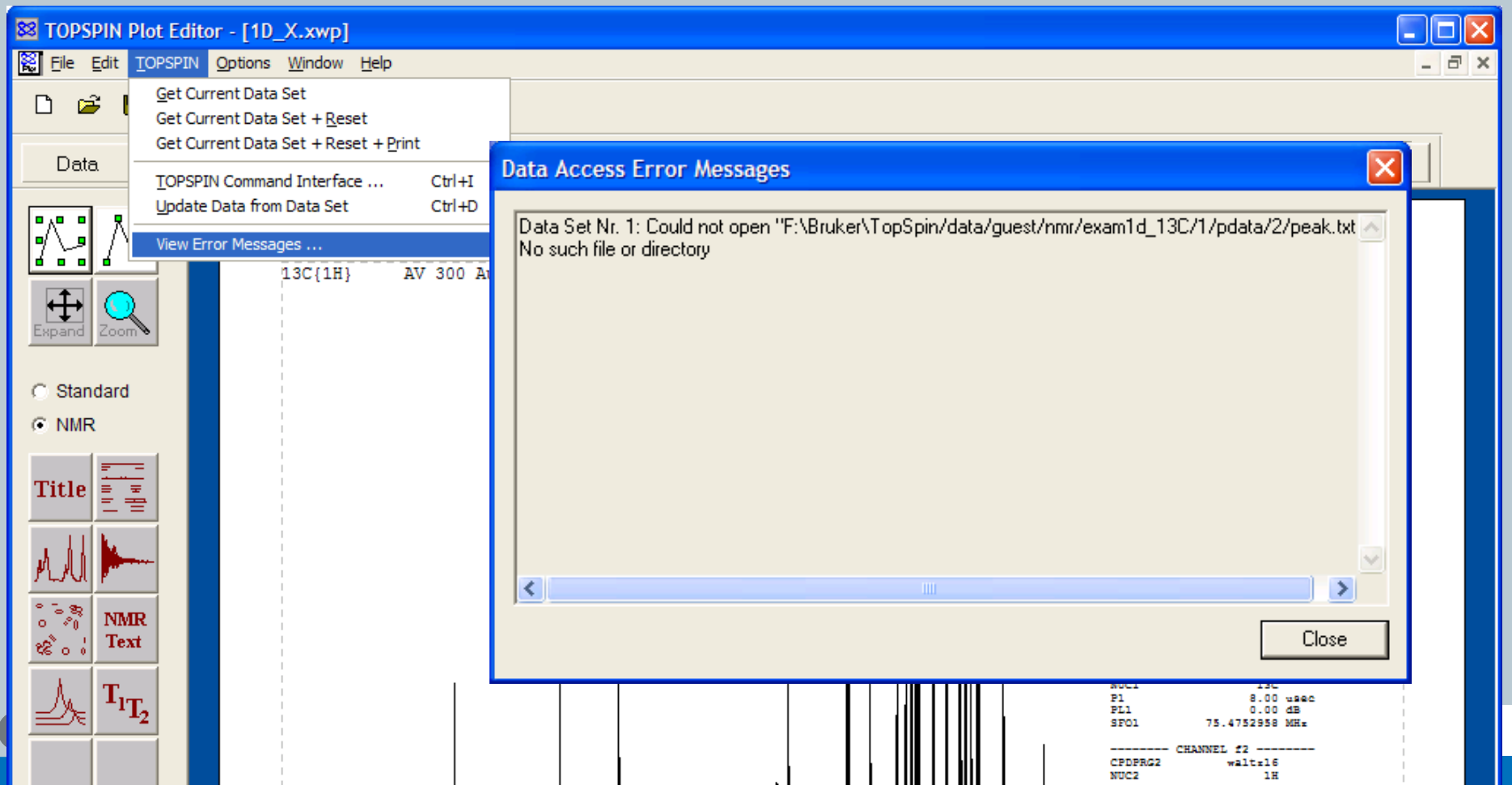
Content


General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

Plot Editor warning messages

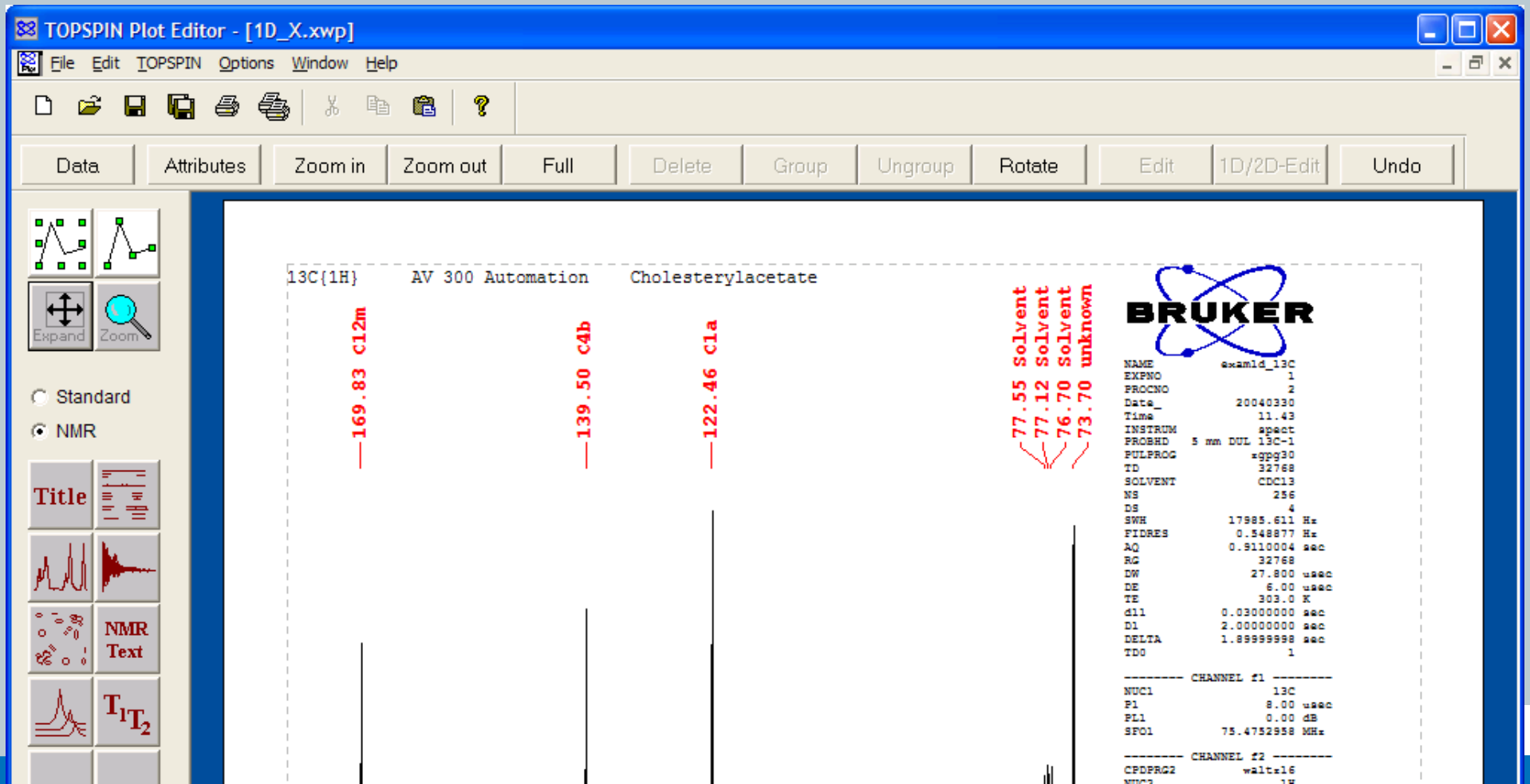
Plot Editor offers a new menu entry which contains a list off all warnings that have been given by the program.

New messages are discrete shown in status line.



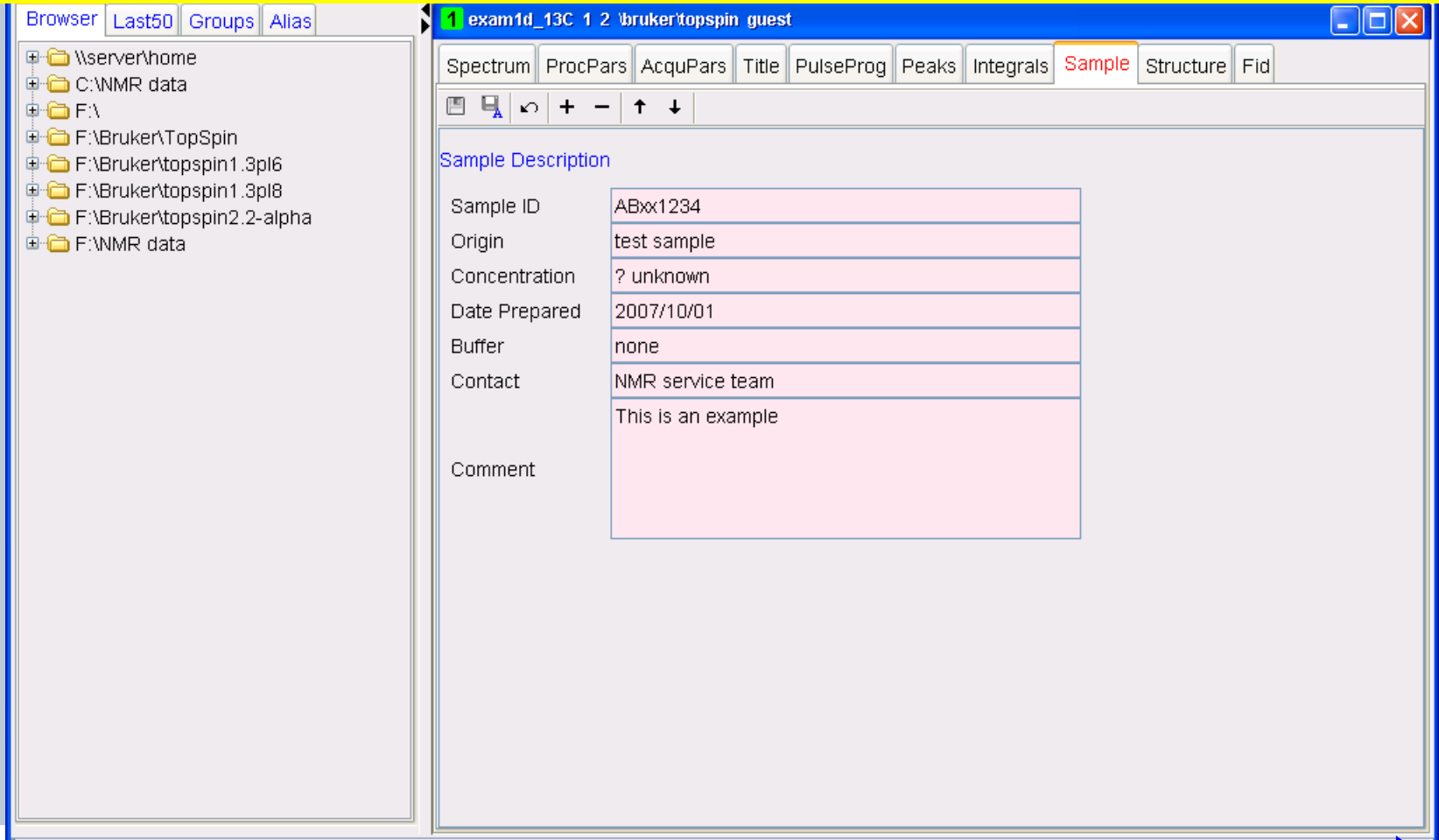
Plot Editor shows annotations

Plot Editor can now be configured to show position (Hz/ppm) or annotations (if available) or both.



Plot Editor shows sample info

Plot Editor Layouts can now be configured to show sample info defined in TopSpin.



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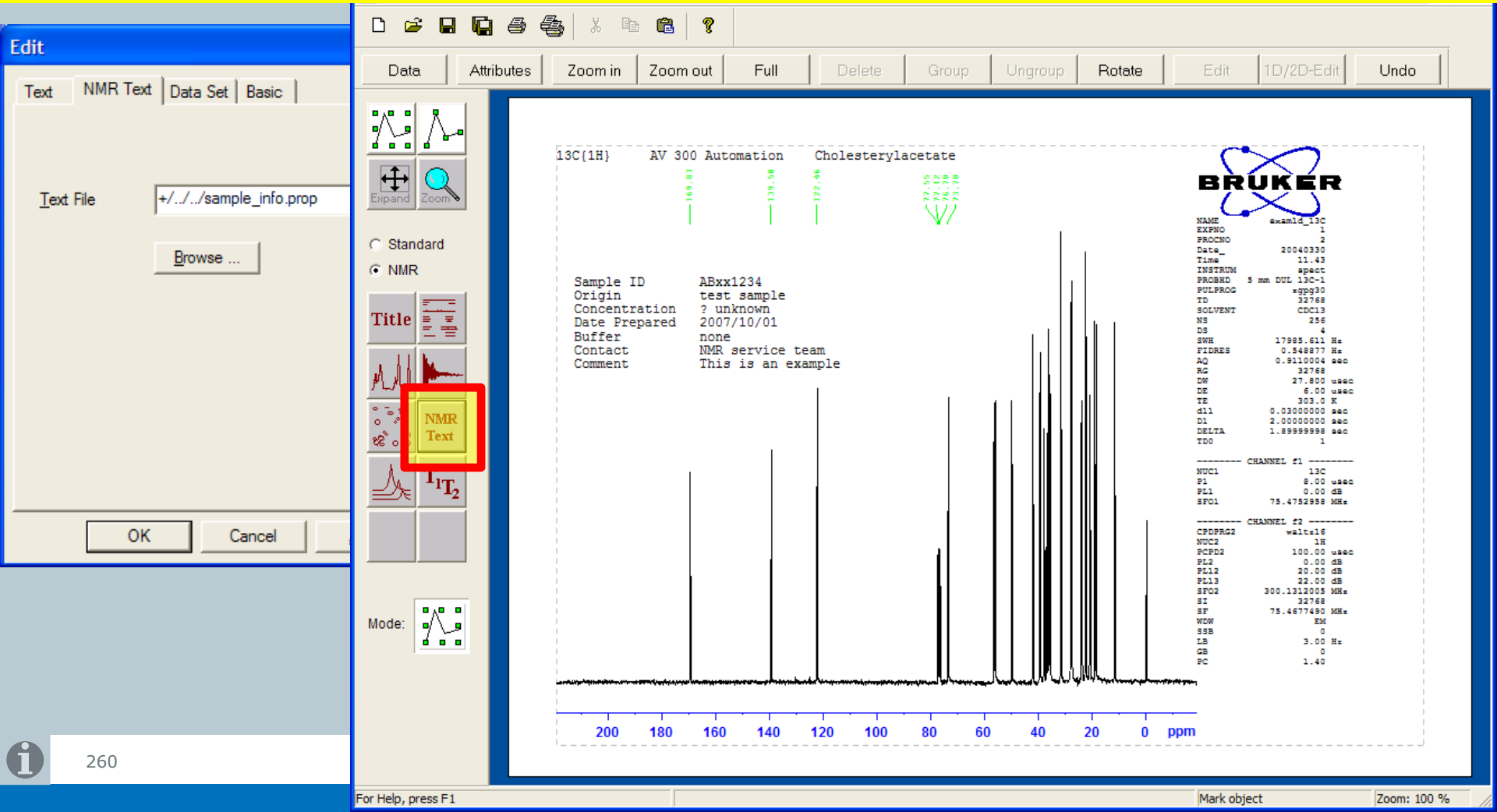


Plot Editor paper formats

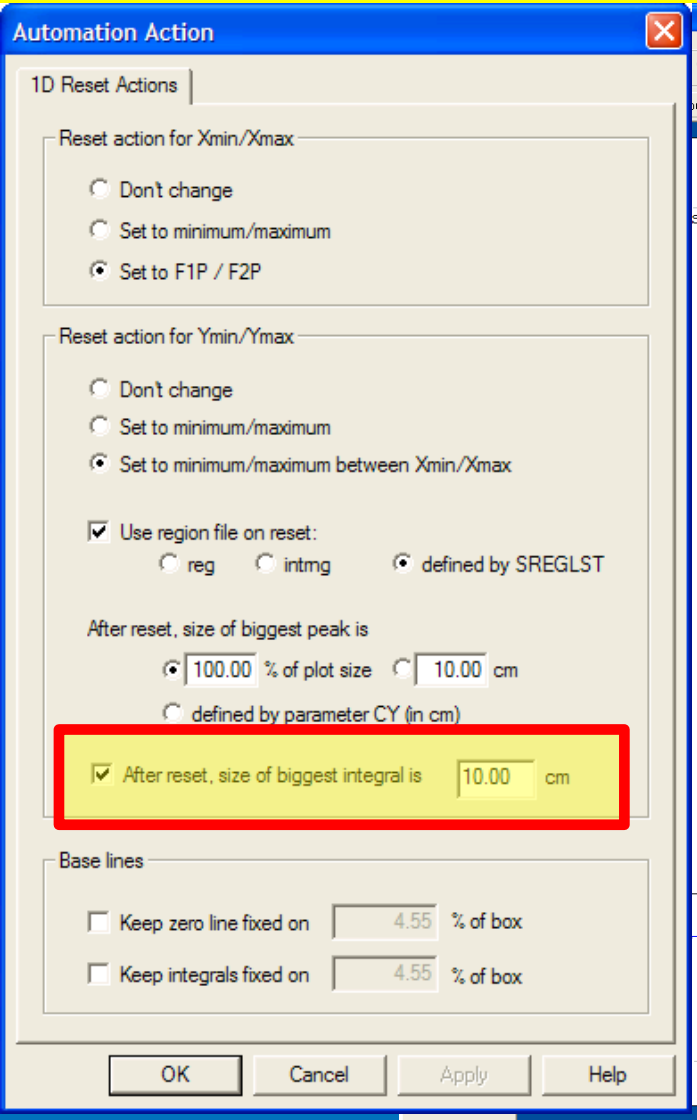
Plot Editor now supports customized paper formats on Windows printers.

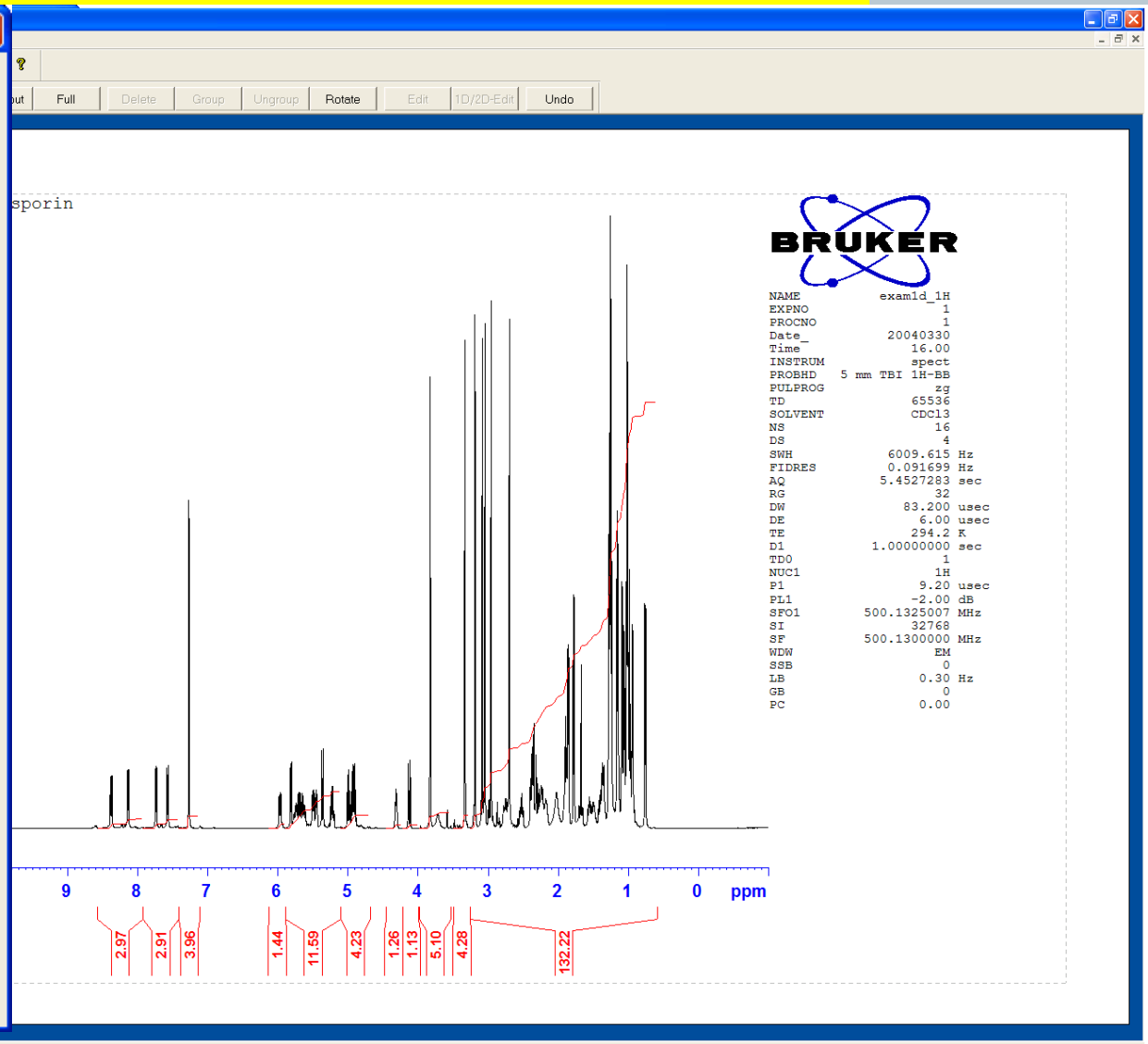
New formats simply need to be defined using the „Printer → Server Properties“ mechanism as provided by Windows itself.

Integral reset action

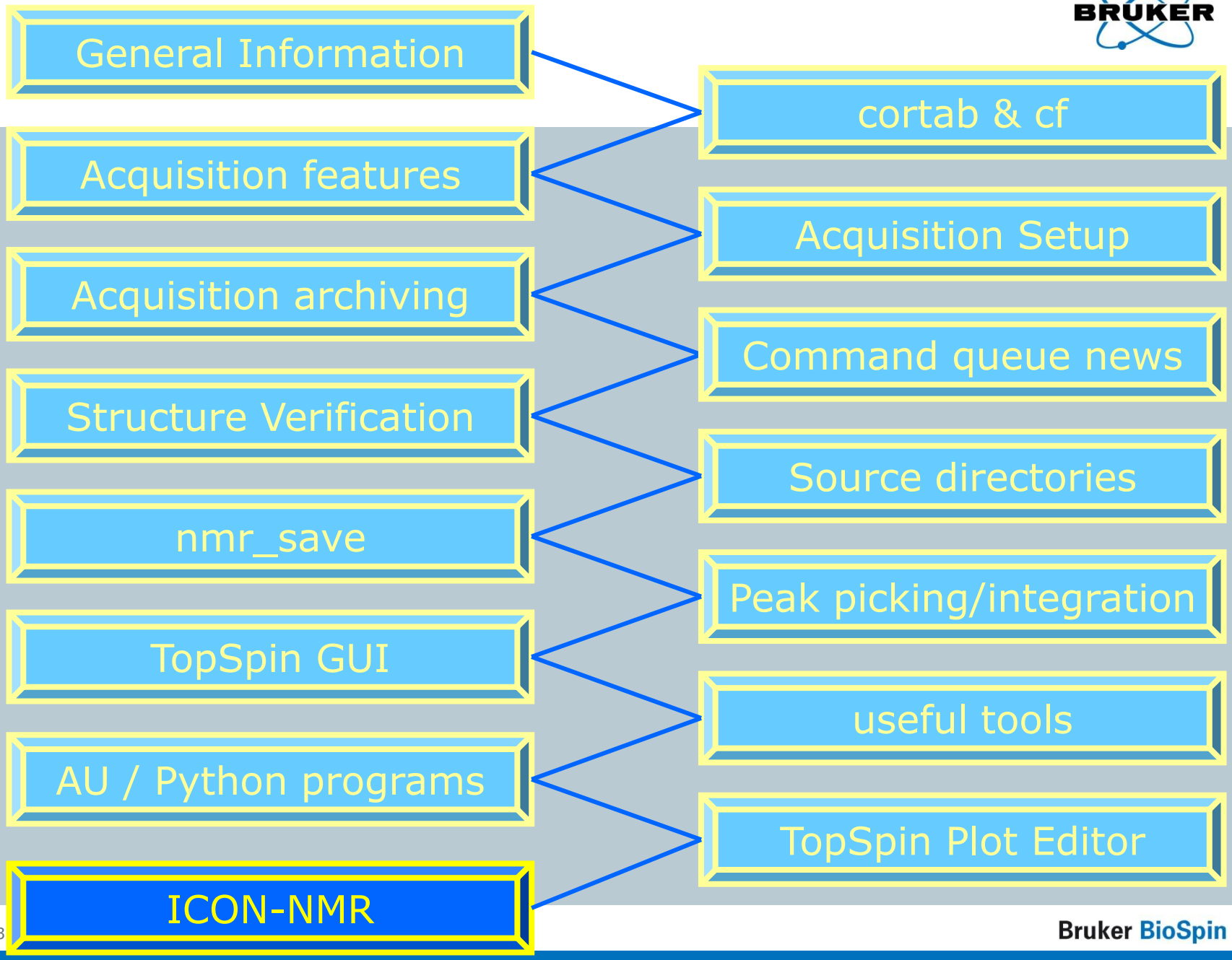
A new reset option for integral height is offered:

After reset size of biggest integral is: [ ] cm





Content

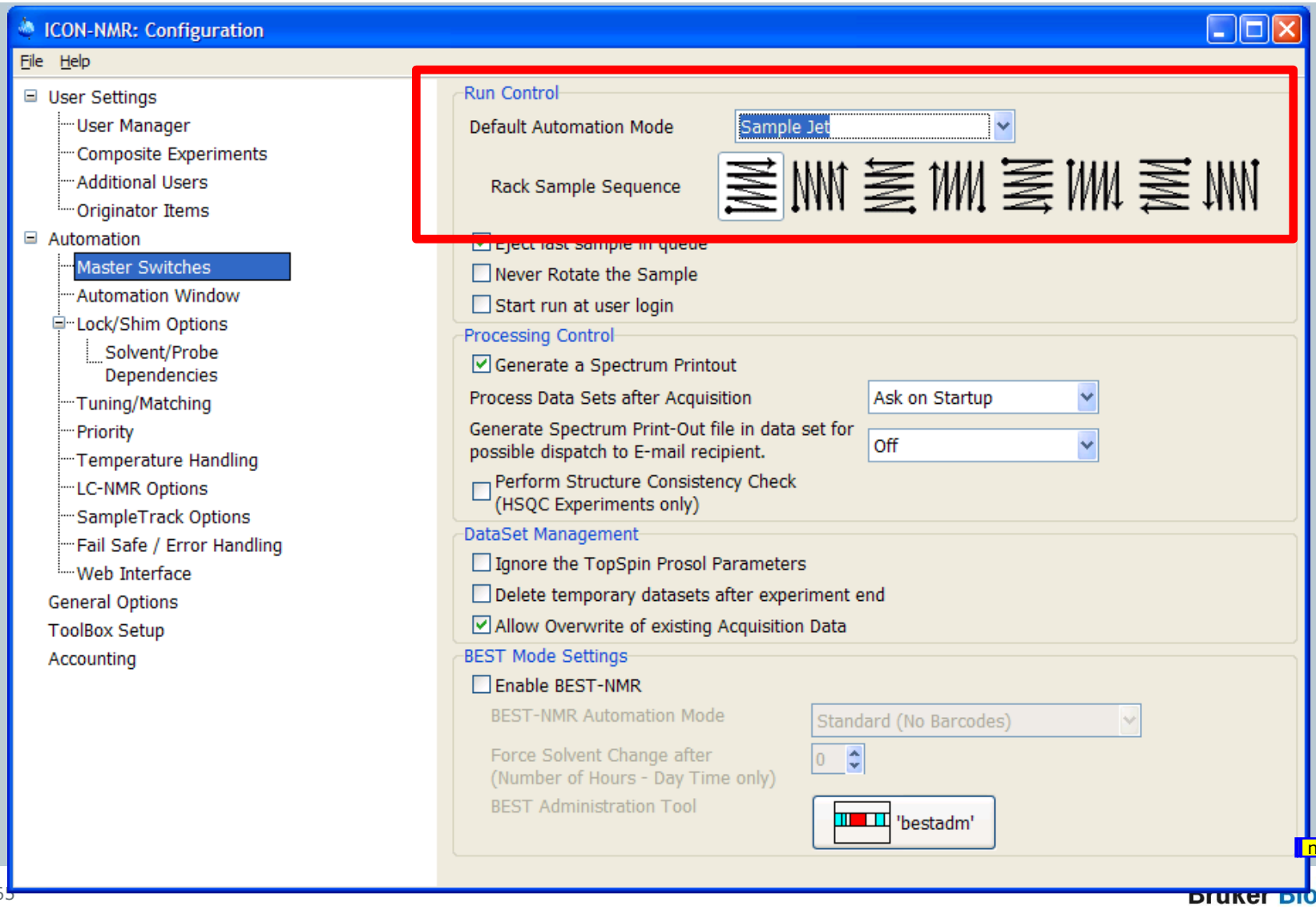

General Information
Acquisition features
Acquisition archiving
Structure Verification
nmr_save
TopSpin GUI
AU / Python programs
ICON-NMR
cortab & cf
Acquisition Setup
Command queue news
Source directories
Peak picking/integration
useful tools
TopSpin Plot Editor

ICON-NMR 4.2 – SampleJet support

Icon 4.2 includes support for the new Bruker SampleJet Sample Changer.
A dedicated Sample Holder overview window along with a configuration option to control the measurement sequence order of experiments is provided. The Automation driver routines have also been optimized to take full advantage of the improved performance.
Icon also fully supports the interfacing of this new unit to the SampleTrack Laboratory Management software.

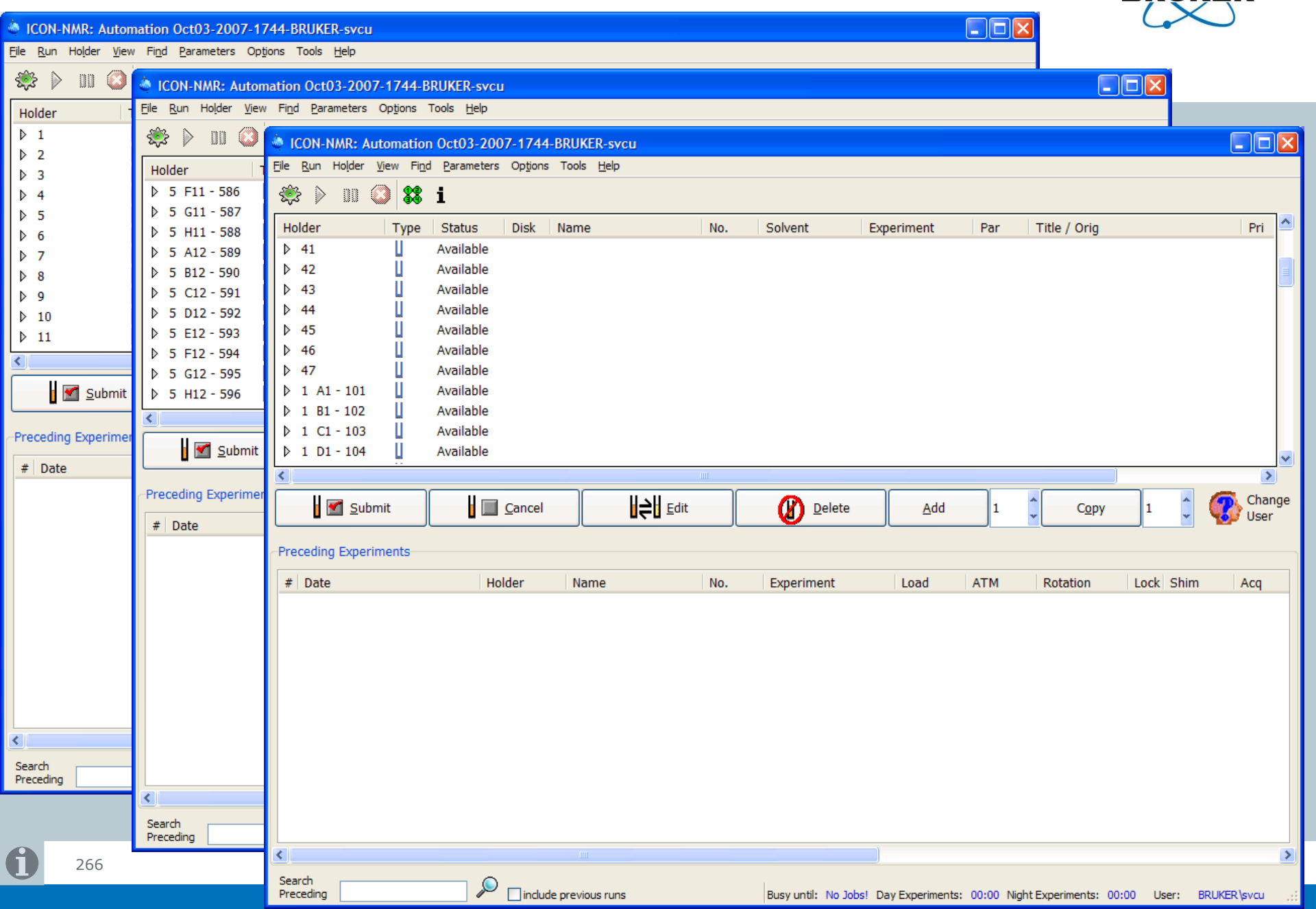
next page

ICON-NMR 4.2 – SampleJet support



next page

ICON-NMR 4.2 – SampleJet support

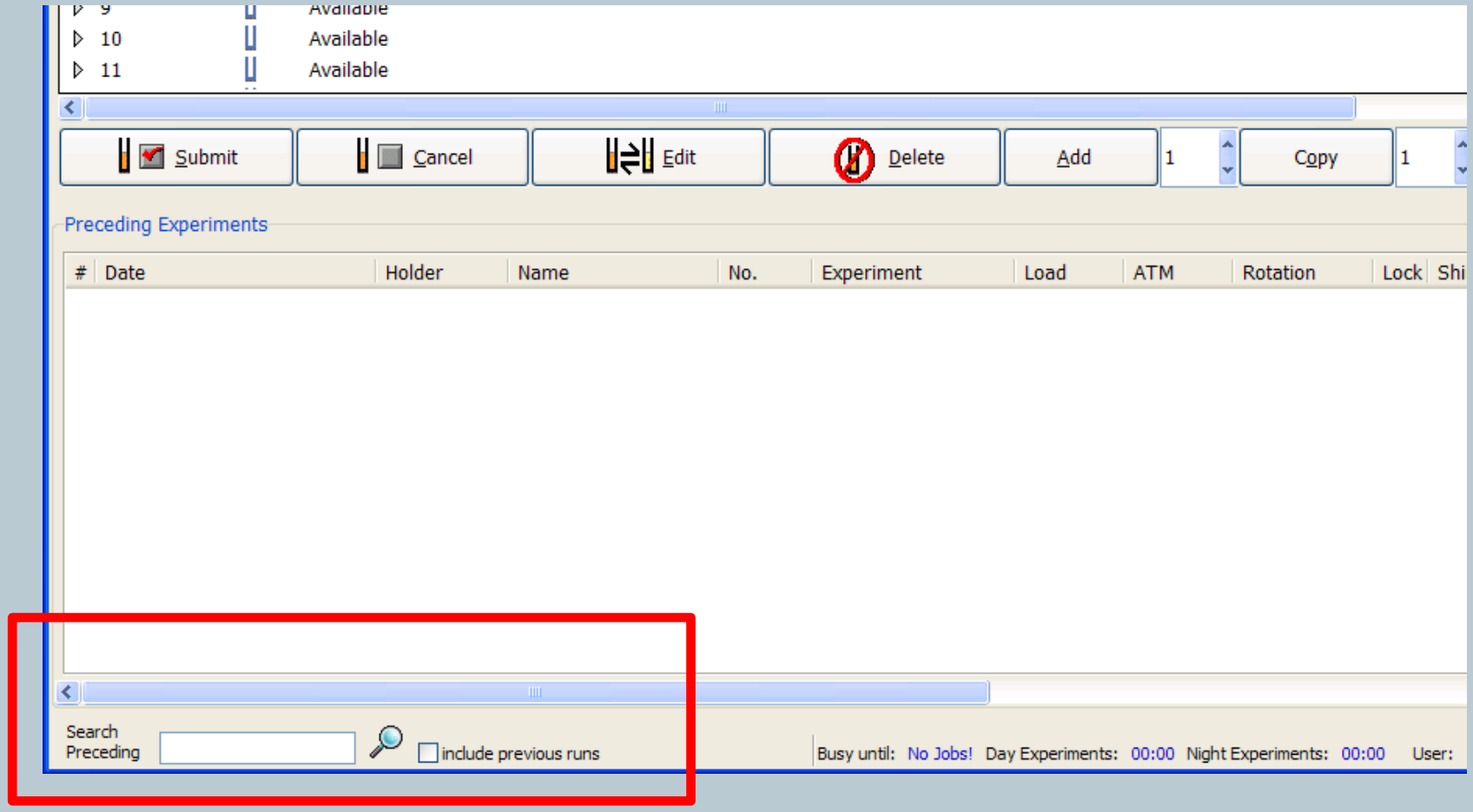


Search history files

A convenient search tool has been added to search all entries from preceding experiments performed within Icon-Nmr. Search for multiple items in an experiment's title text, dataset name or a particular remarks message. A list of items is generated in the same manner as the Preceding Experiments (history) list which may be then used to navigate under TopSpin or Amix Viewer to the respective dataset.

next page

Search history files



Web-Icon Improvements

Experiments may now be remotely edited via the Web interface.

A timeout feature has also been added to logout idle web users, improving security and throughput.

ICON-NMR 4.2 – Remarks fields

Remarks field now shows process messages

Should any procedure generate an error or warning during sample measurement, a copy of the text of the warning or error will appear in the “Remarks” column of the Preceding Experiments (history) list.

Failsafe watchdog timer

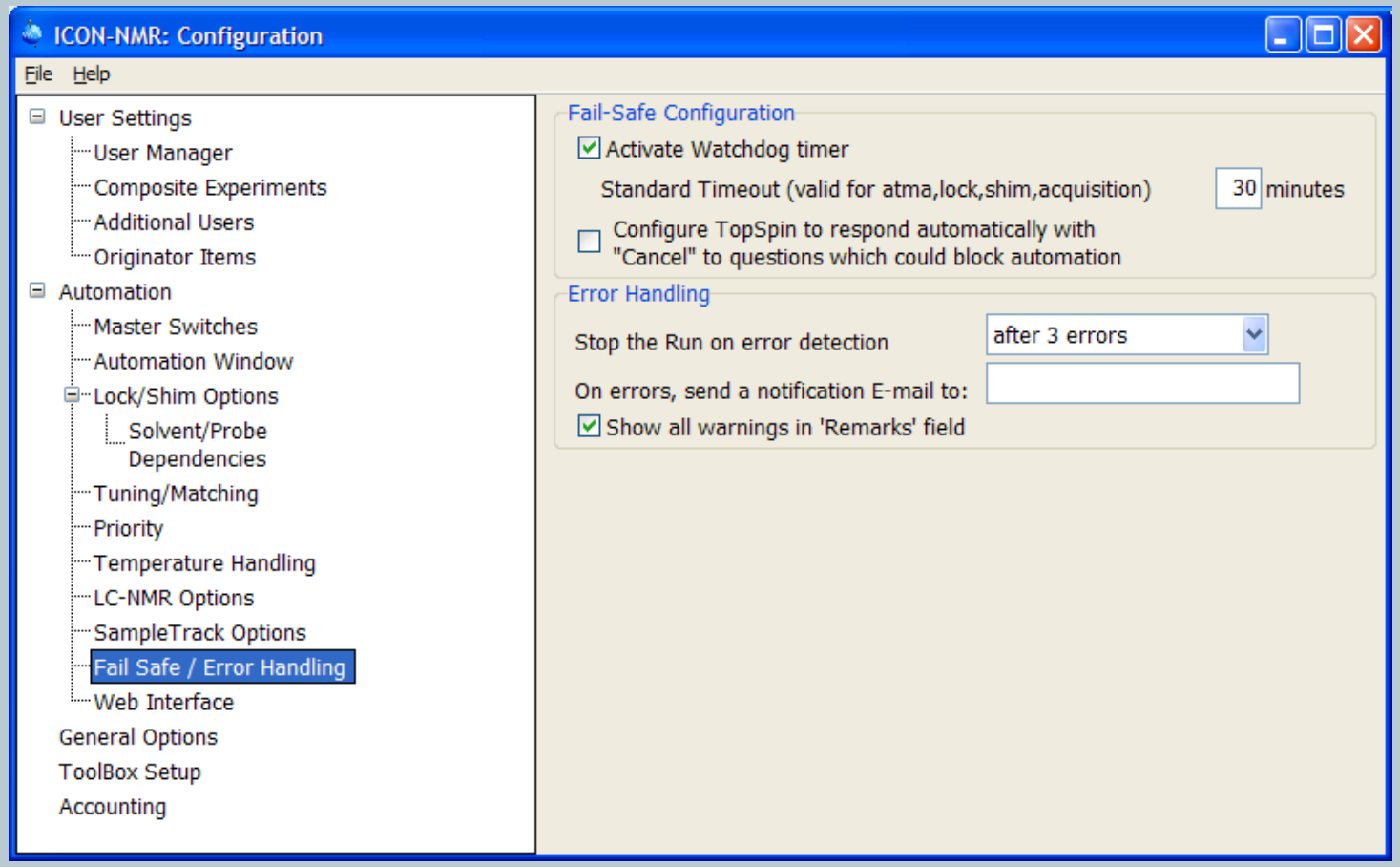
If any action takes longer than expected during the automation process, the run will be restarted. The action which failed to complete will be also restarted, but if it fails again, it will be skipped.

The Automation run will no longer be blocked by any processes which fail to respond.

The time allotted for waiting may be configured and where necessary this system may be circumvented.

next page

Failsafe watchdog timer



ICON-NMR 4.2 – zip archive

Zip copy, Zip data mail (User Manager) permission

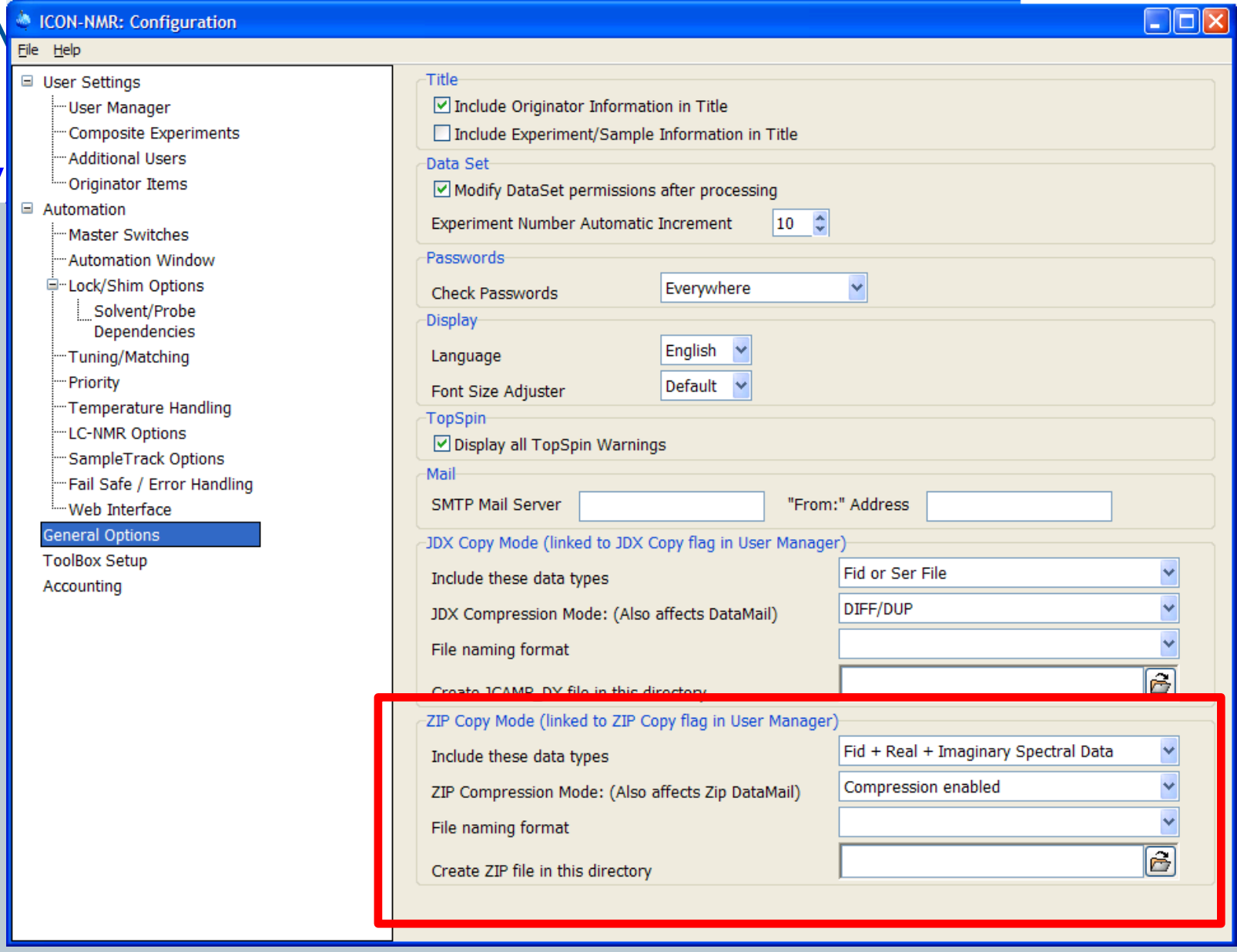
Icon can now generate Zip files of the generated datasets as part of the run. These can be emailed in the same manner as JDX files have been up to now.

Zip Files may also be copied to a particular directory if required, in the same manner as the JDX-Copy mode.

next page

ICON-NM

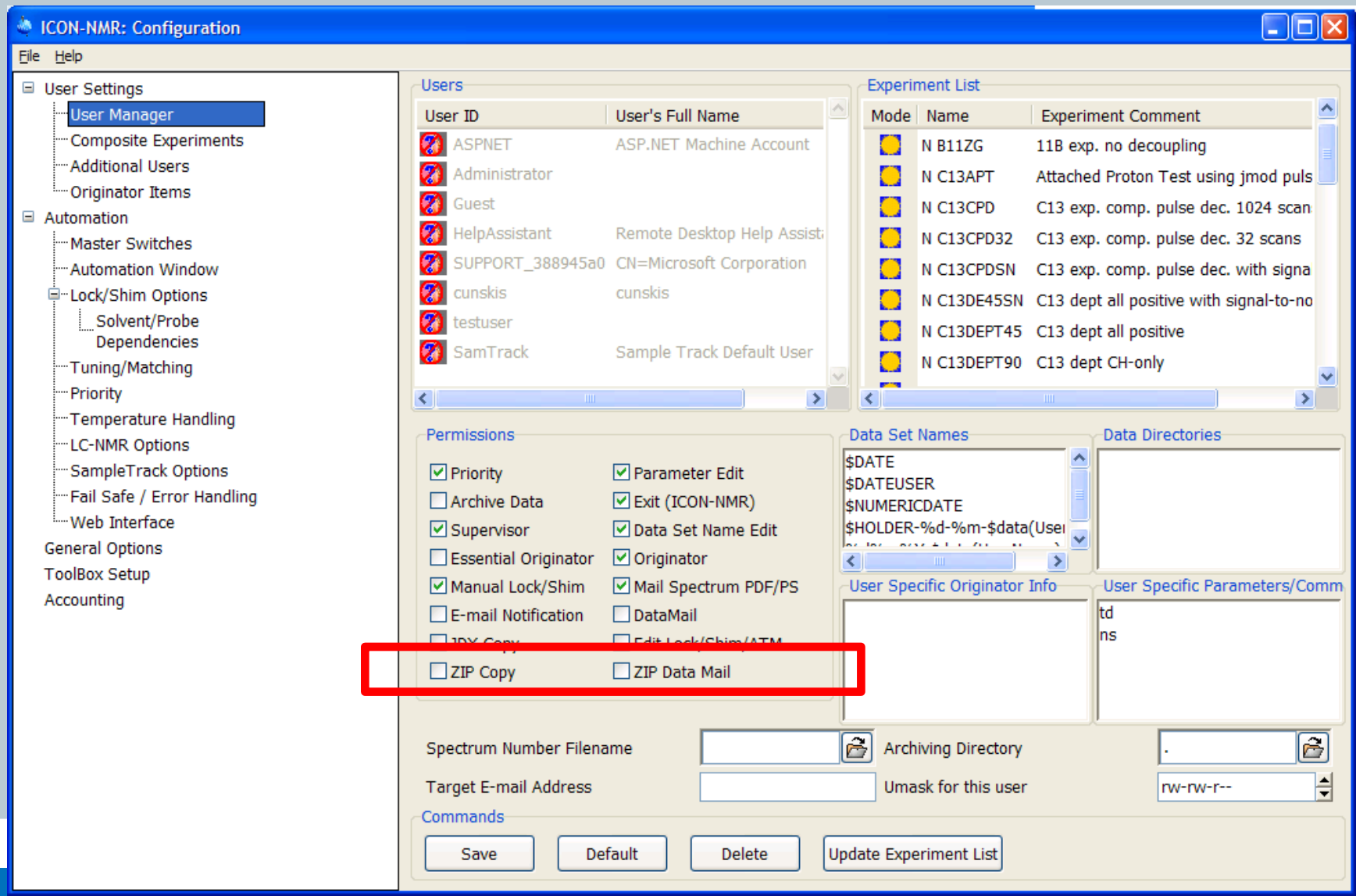
Zip copy



next page

ICON-NMR 4.2 – zip permissions

Zip copy, Zip data mail (User Manager) permission



ICON-NMR 4.2 – regular expressions

Originator ‚Regular expression' check

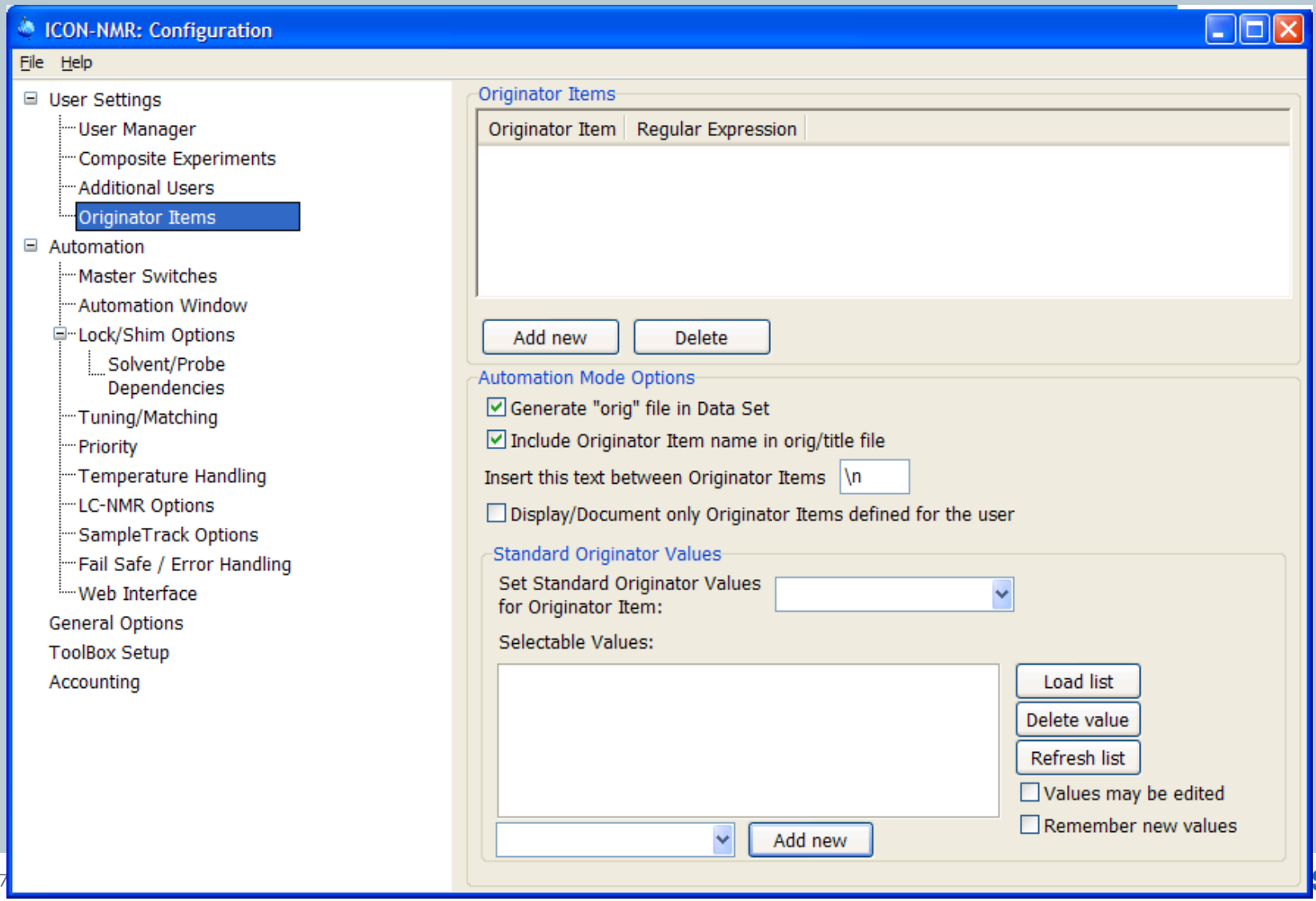
Originator item information may be screened according to syntax rules.
This will further reduce the likelihood of incorrect sample information being entered when samples are being submitted.
More information on how to use/set up 'regular expressions' can be found e.g. here:

http://www.regular-expressions.info

next page

ICON-NMR 4.2 – regular expressions

Originator Regular expression check



Experimental Form Style entry mode

This method of submission may be useful when the instrument is working in environments where access to the instrument needs to be streamlined.
Here the sample position, dataset name and experiment number is set automatically (using either the Spectrum Number Filename or User Manager Dataset Name entry).
All that remains is for the user to set Solvent and Experiment and Title/Originator Info.

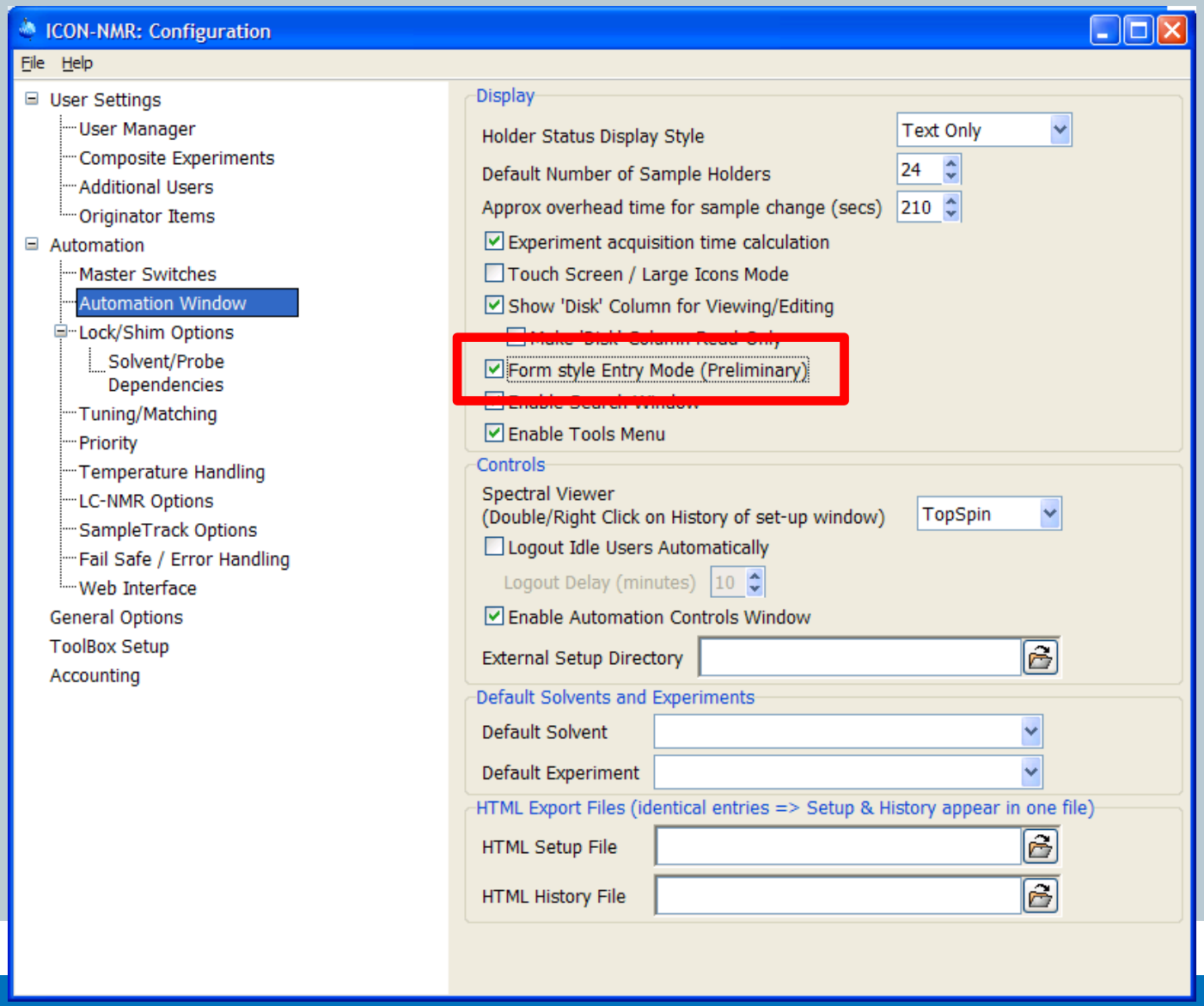
Comments on this new system please to

nmr-software-support@bruker.de

next page

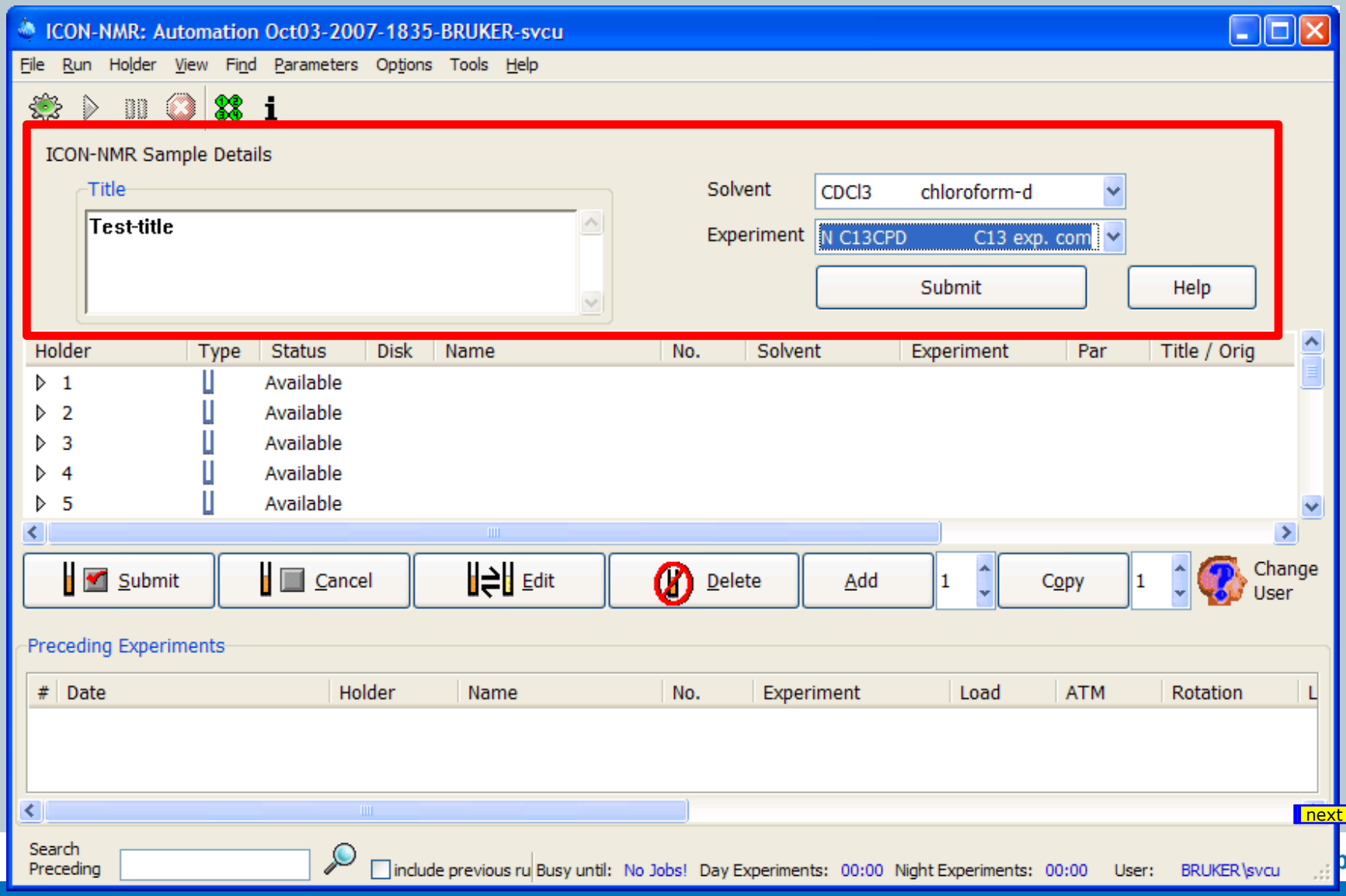
ICON-NMR 4.2 – automation setup

Experimental Form Style entry mode



ICON-NMR 4.2 – automation setup

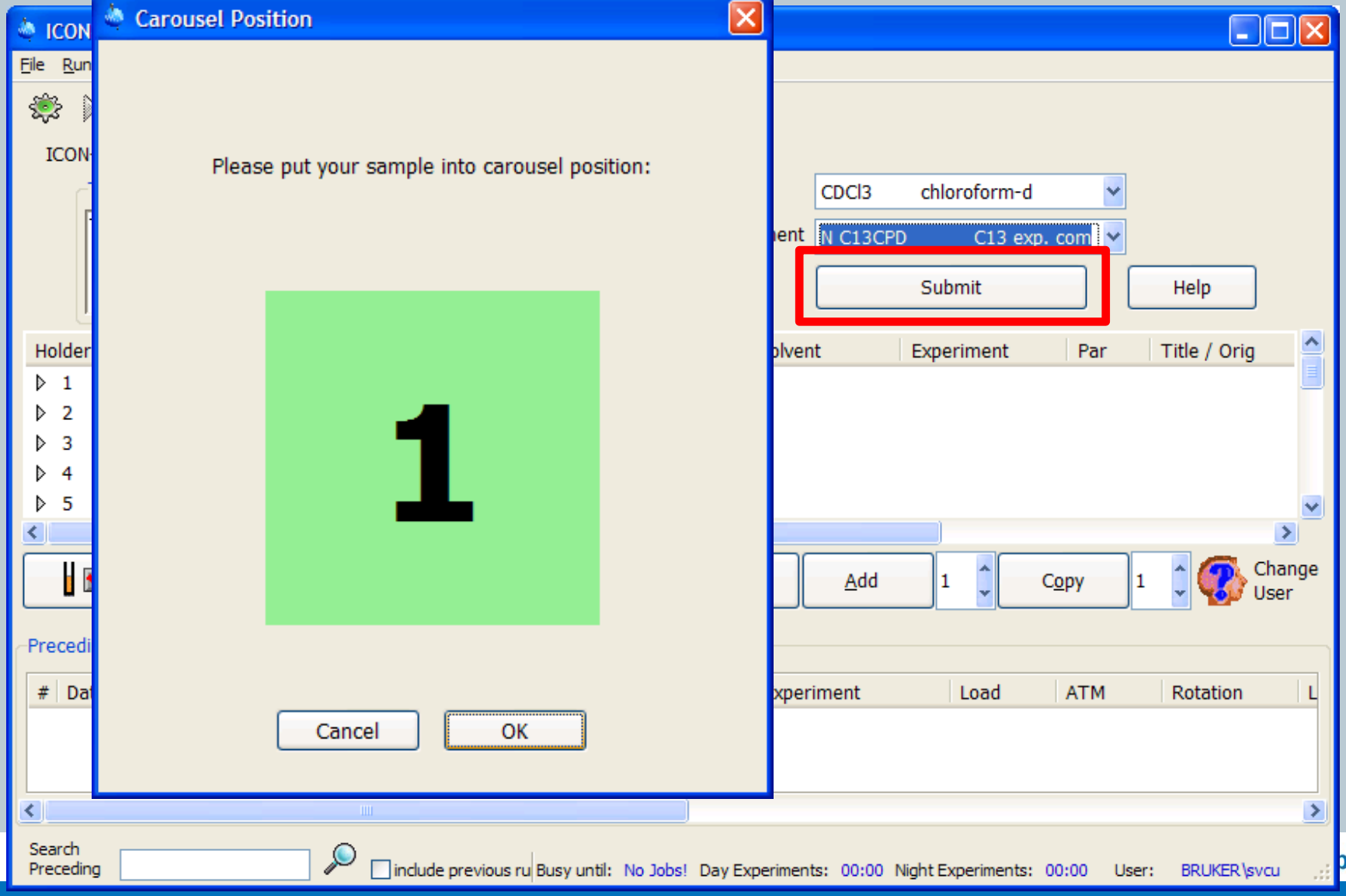
Experimental Form Style entry mode



next page

ICON-NMR 4.2 – automation setup

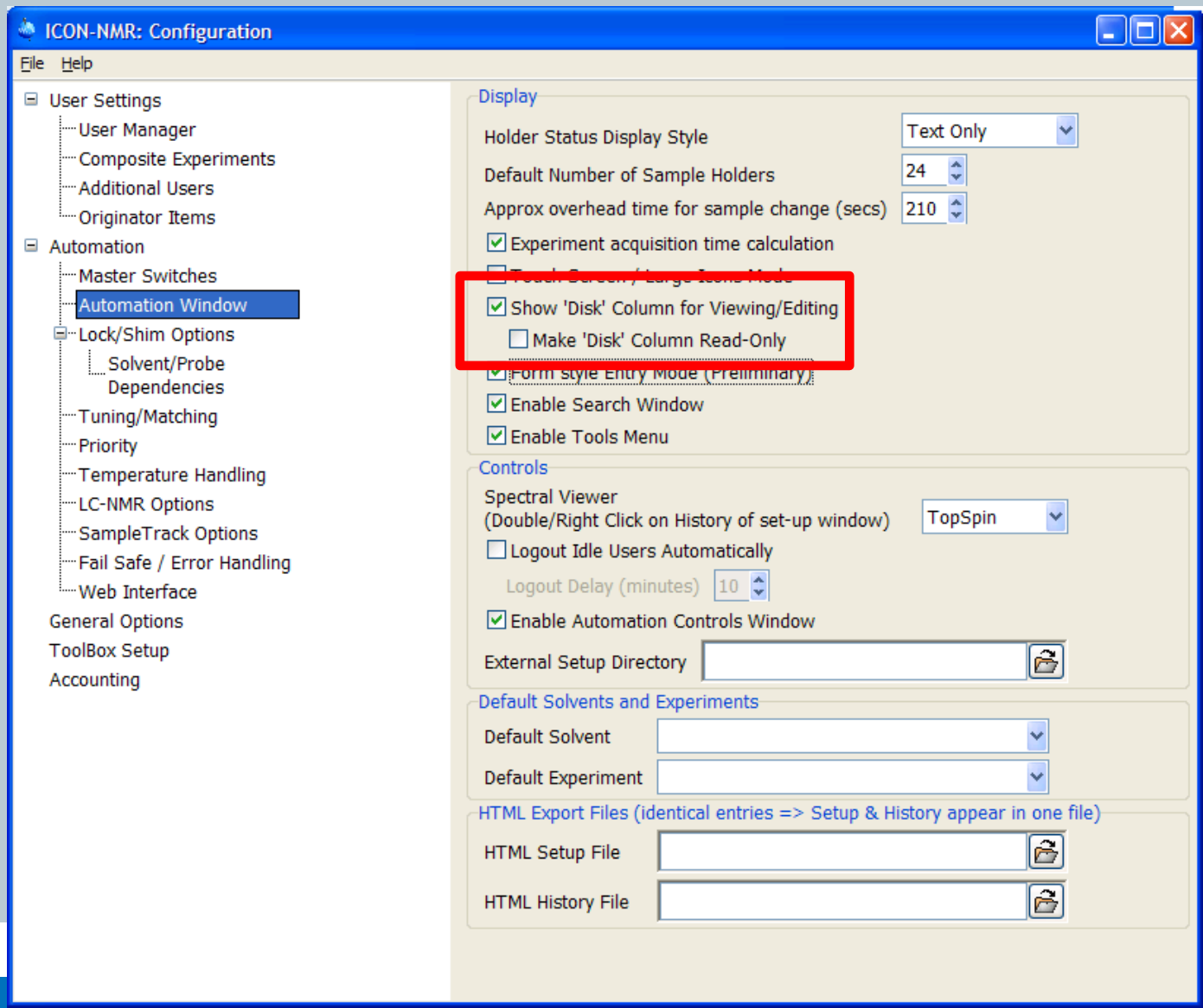
Experimental Form Style entry mode



ICON-NMR 4.2 – automation window

Disk column …

… can be hided optionally.

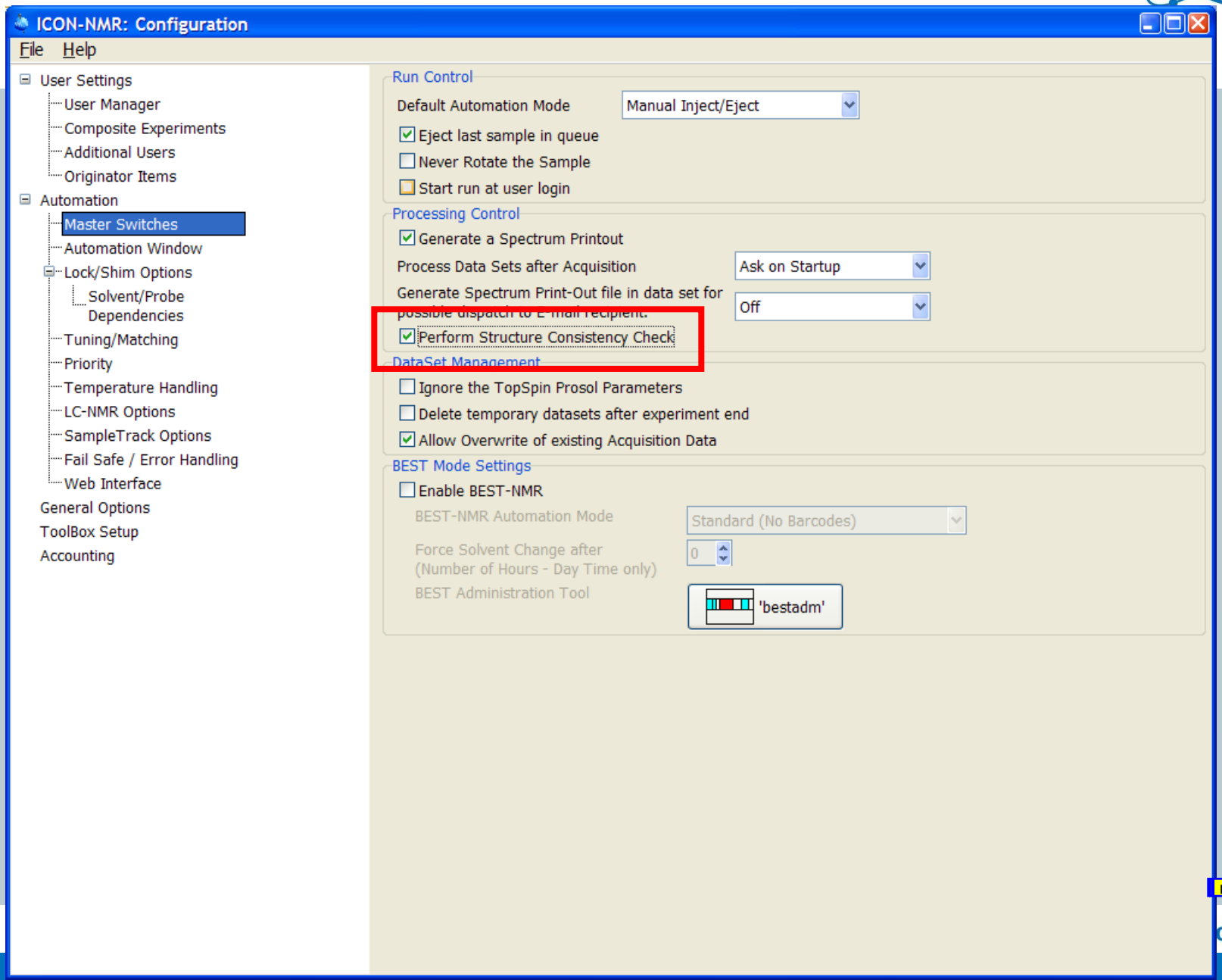


Structure consistency check

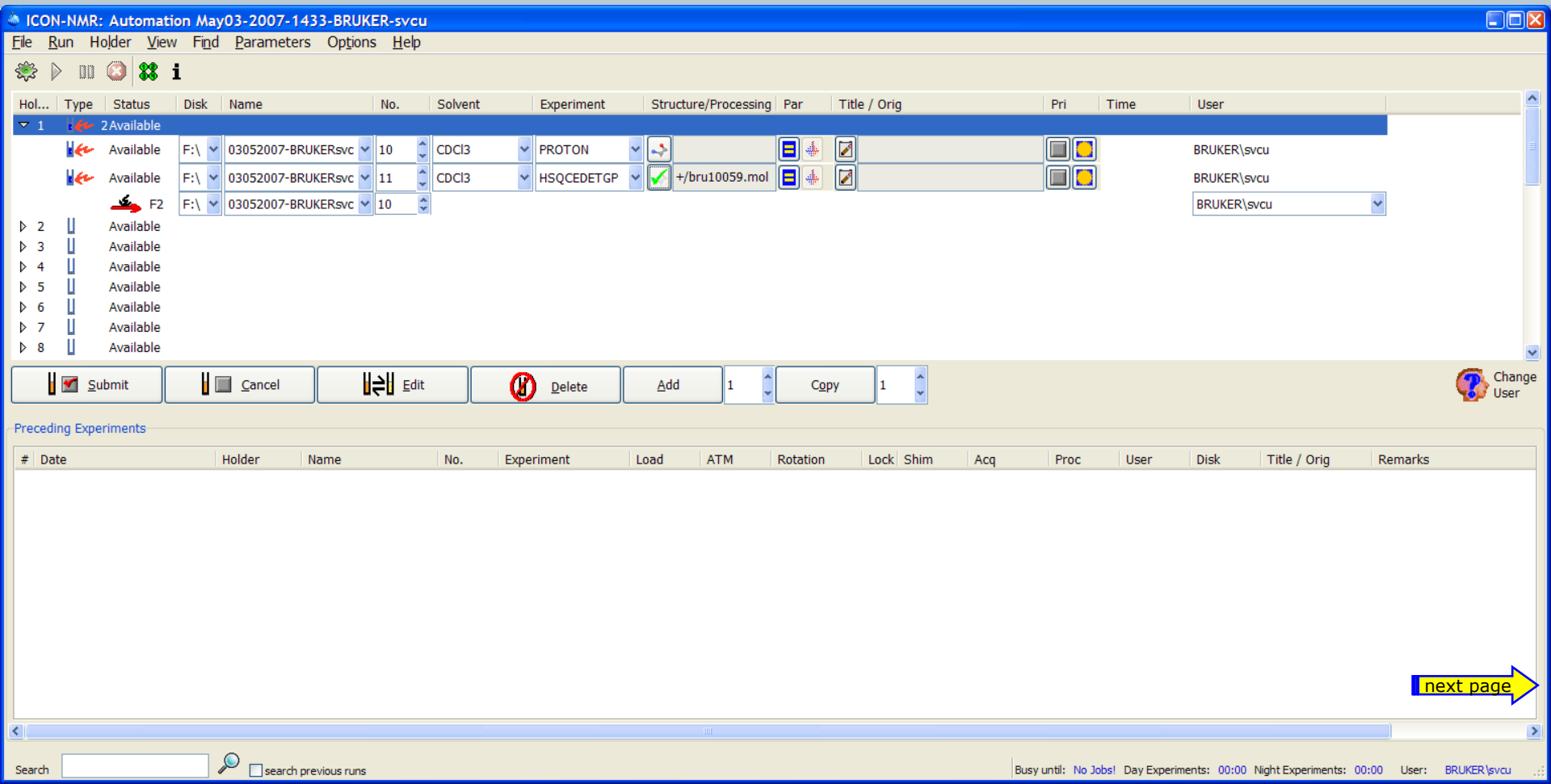
An additional entry field may optionally be added to the Automation window where a Mol/SD file may be set which will be used on HSQC experiments to perform an automated structure consistency check.
This feature requires the Perch Software Tools.

next page

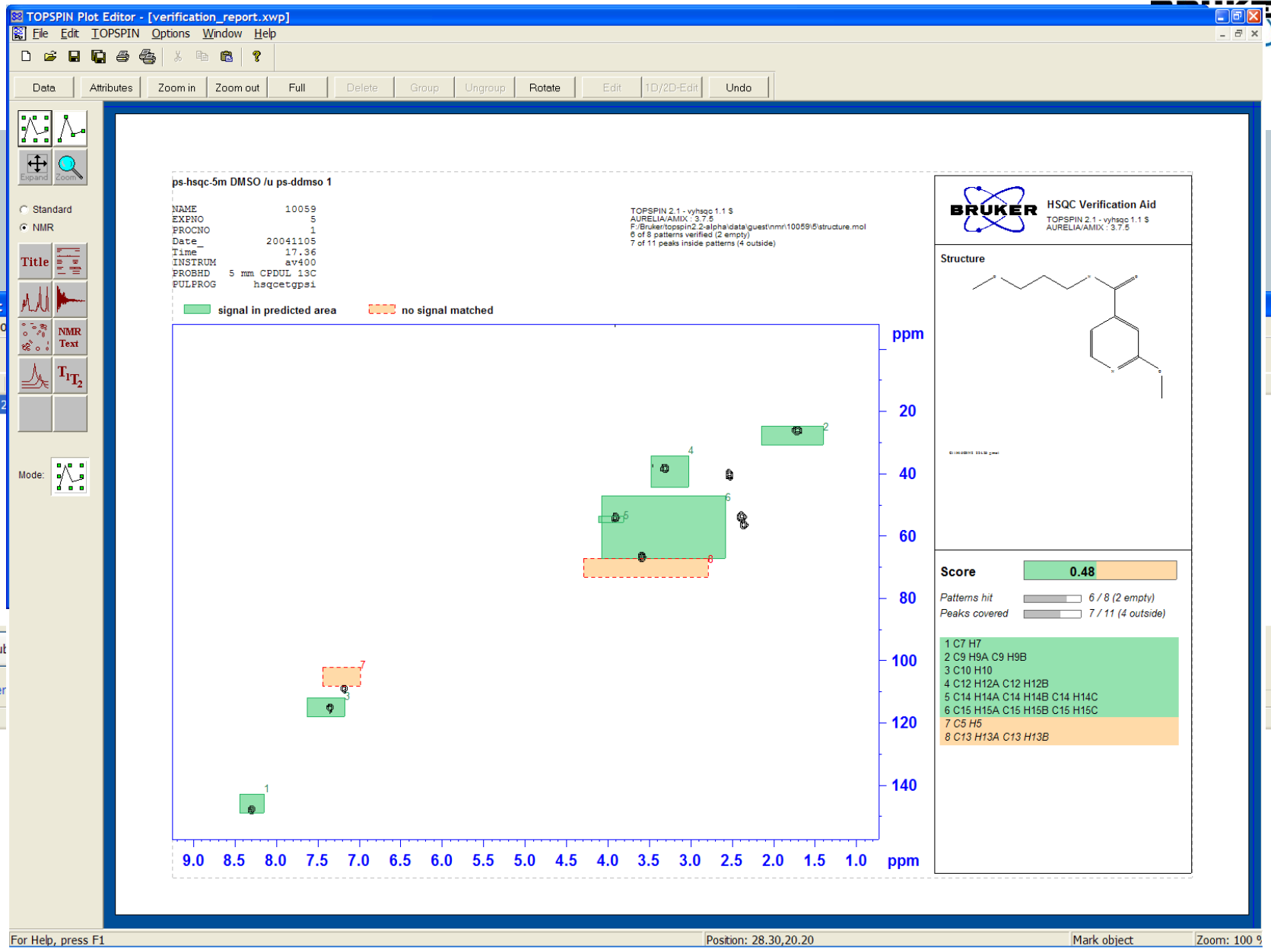
ICON-NMR 4.2 – structure verification aid



ICON-NMR 4.2 – structure verification aid



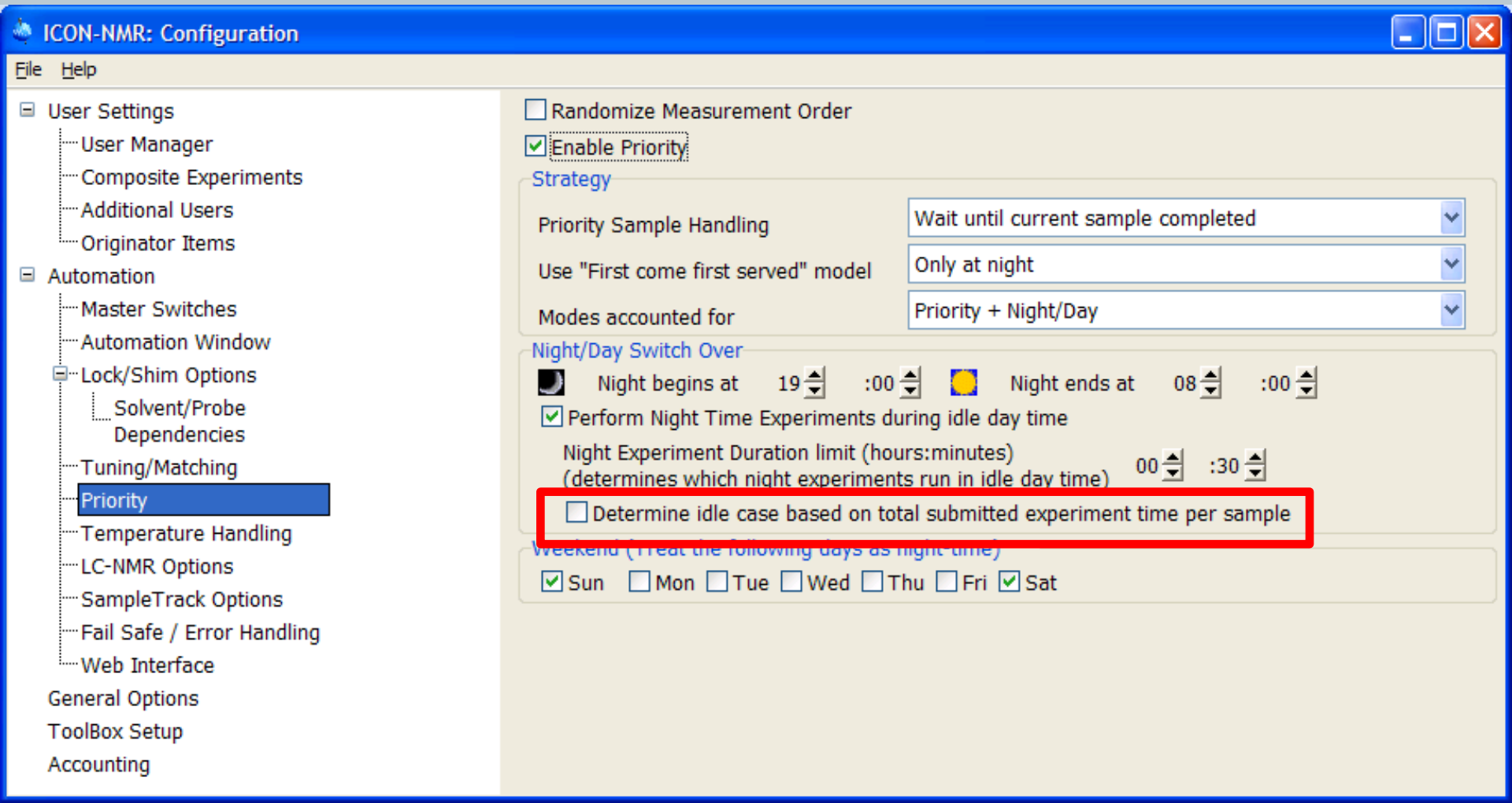
ICON-NMR 4.2 – structure verification aid



ICON-NMR 4.2 – priority

Night time experiments …

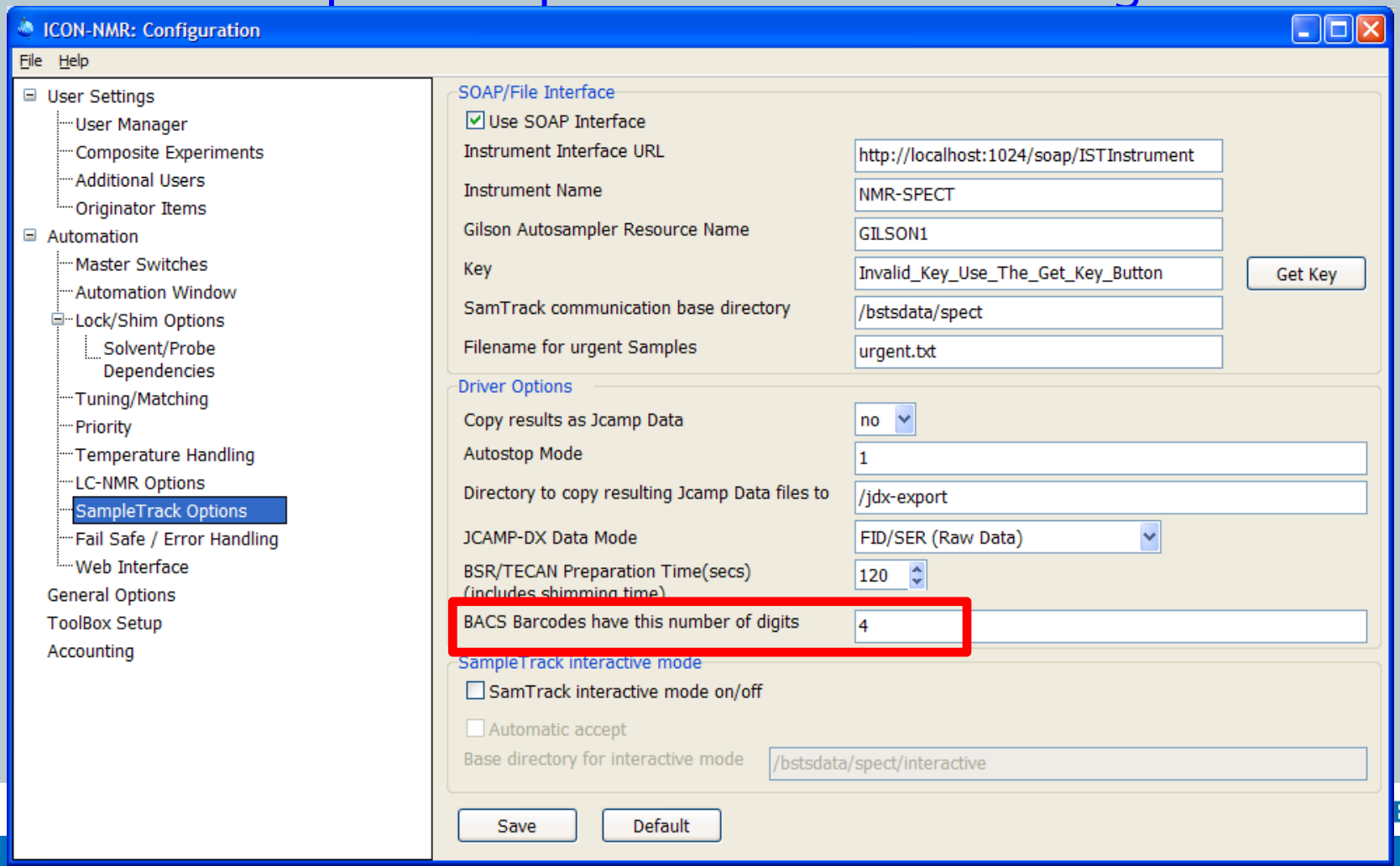
…may now be treated as single entities when determining whether they should be run in idle instrument time.



ICON-NMR 4.2 – bar code

BACS bar code reader

ICON-NMR can be configured that the BACS bar code reader will expect a specified number of digits to read.



ICON-NMR 4.2 – Toolbox

Toolbox/BioTools …

… contains a new updated default Bio Experiment definition file, with lots more experiments.

ICON-NMR 4.2 – automation setup

Spreadsheet Import …

… allows to specify that the sample position will be taken from a particular column of the sheet.

ICON-NMR 4.2 – new keywords

External Setup Files …

… may contain new keywords:

- NIGHT for night experiments and
- MOLFILE to perform the Structure Consistency Check with a particular Molfile.

ICON-NMR 4.2 – history available

History of previous experiments …

… offers new “Load” column, depicts whether a sample was inserted into the magnet correctly or not.

ICON-NMR 4.2 – no hick-up

Questions …

… issuing from TopSpin may be automatically answered with an automatically generated “Cancel” click, thus preventing any Automation Lockup when no operator is present.

ICON-NMR 4.2 – Import from TopSpin

Import any experiment/dataset directly into the Automation window

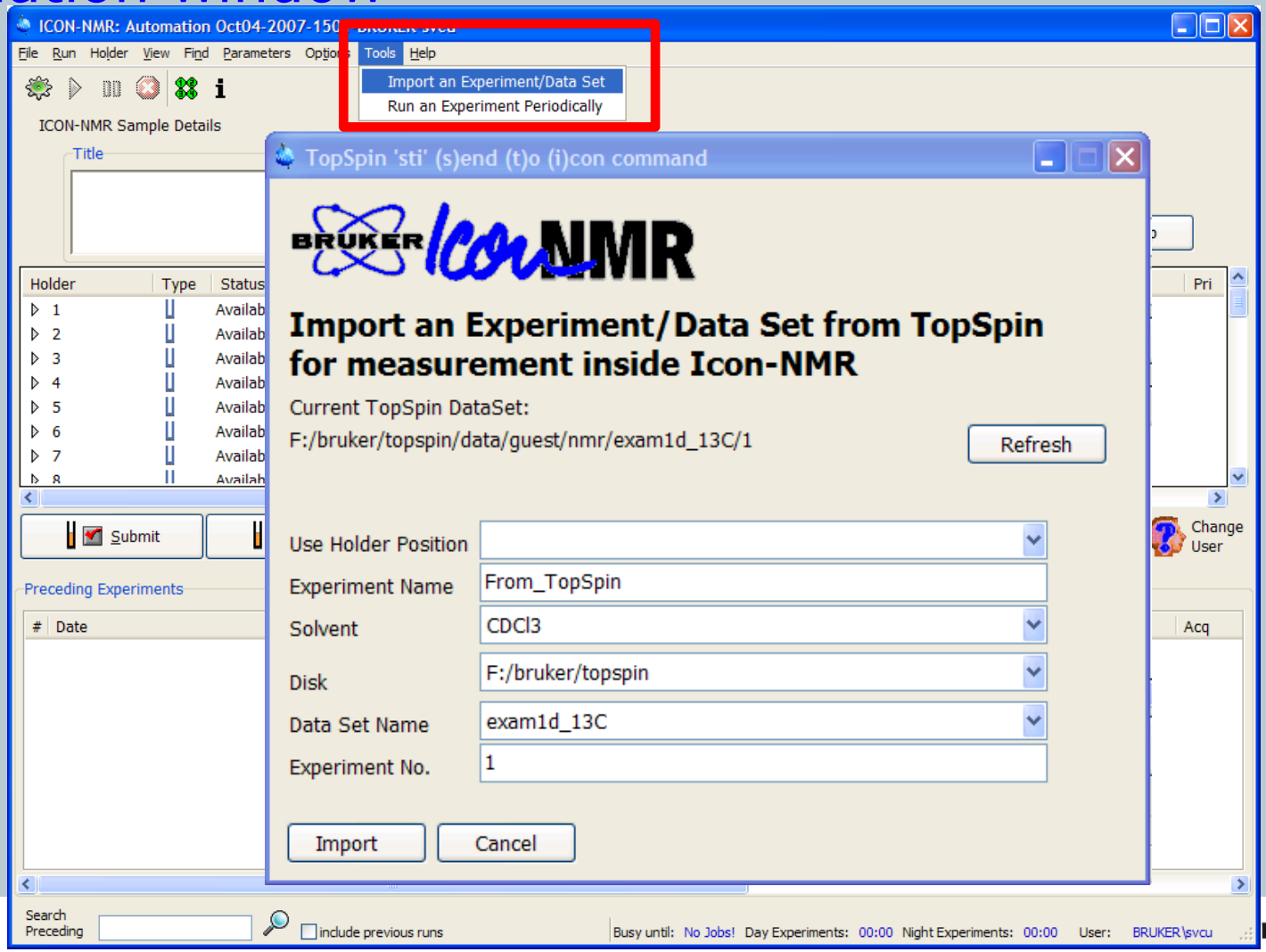
Set up a dataset as you like it in TopSpin and have this dataset sent to Icon-Nmr for measurement inside ICON's Automation interface on any sample.

The dataset may be sent to icon directly from TopSpin using the **sti** (send to icon) command.

next page

ICON-NMR 4.2 – Import from TopSpin

Import any experiment/dataset directly into the Automation window



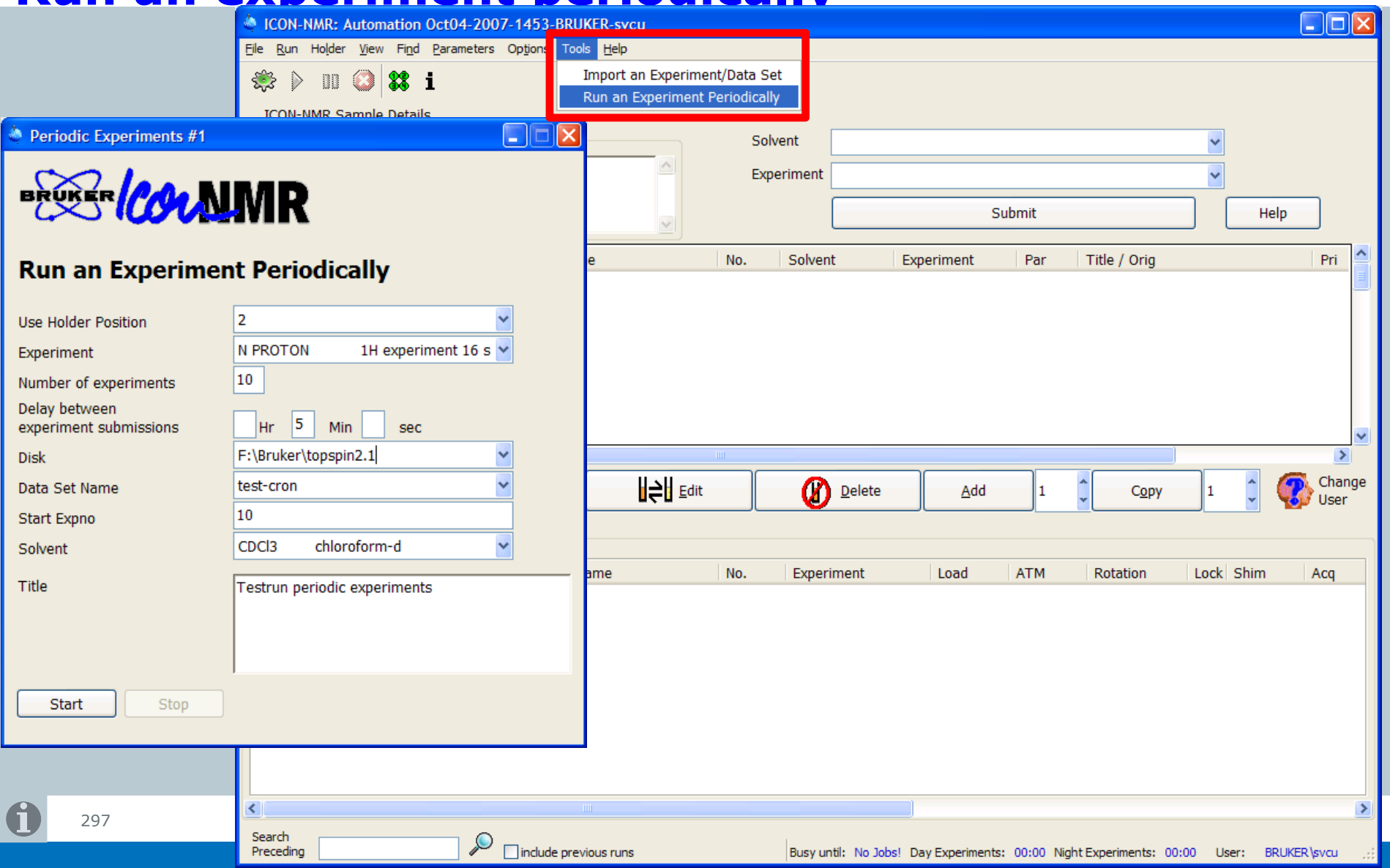
Run an experiment periodically

Up to 10 different experiments (including composites) may be queued for automatic periodic submission on any sample. Queue an experiment to run any number of times. The experiments will be submitted automatically at regular intervals and run with the priority flag set.

next page

ICON-NMR 4.2 – periodic experiments

Run an experiment periodically



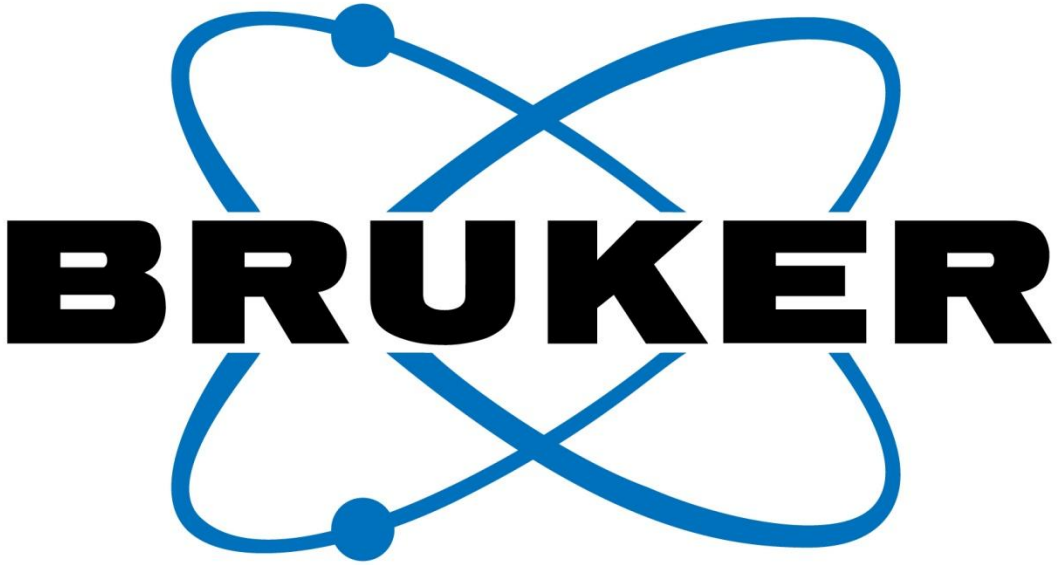
ICON-NMR 4.2 – look and feel

Color/Theme support under Linux

Change the colors used and look and feel of ICON-NMR directly from the Linux Desktop Control Panel.
Icon will adopt the standard look and feel of other programs running under Linux.
Windows Users will also notice more conformity with the desktop settings.

Mouse behaviour

On Microsoft Windows, the Mouse will jump to default buttons automatically when this mouse option has been activated in the “Control Panel”.



www.bruker-biospin.com

??Picture digital resolution